Class Notes in Discrete Mathematics, Operations Research, Statistics and Probability (Fourth Edition, v1)

Goodwin, Roger L

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Edited by Roger L. Goodwin

Summit Point, WV 25446

Editor's Note: In graduate school, it became too cumbersome for me to look-up equations, theorems, proofs, and problem solutions from previous courses. I had three boxes full of notes and was going on my fourth. Due to the need to reference my notes periodically, the notes became more unorganized over time. That's when I decided to typeset them. I have been doing this for over a decade. Later in life, some colleagues asked if I could make these notes available to others (they were talking about themselves). I did. These notes can be downloaded for *free* from the web site http://www.repec.org/ and can be found in the Library of Congress. Note that the beginning of each chapter lists the professor's name and affiliation. Additionally, the course number, the date the course was taken, and the text book are given. The reader may also notice that I have made more use of the page space than in the previous editions of this manuscript. Hence, the book is shorter. If this causes the reader problems, then simply copy the proofs onto a blank sheet of paper — one line per algebraic manipulation. In this text, I put several algebraic manipulations on one line to save space. I thank Winston for helping typeset the notes.

Winston was born on
October 22, 2003 in Winton Salem,
NC. She died of natural causes on
May 4, 2013 in Summit Point, WV.

Contents

Chapter 1

Discrete Structures

Place: Old Dominion University
Timeframe: Fall Semester, 1987
Instructor: Jane Randall
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Office Hours: Monday: 3:00 - 5:00, Wednesday: 11:00 - 12:00, Friday: 10:00 - 12:00

Course Description: This course will cover a variety of discrete mathematical concepts which have applications in computer science. Topics will include symbolic logic, set theory, binary relations, and functions.

Prerequisite: CS 160

Text: *Discrete Mathematics in Computer Science,* by Stanat and McAllister.
Material to be covered: Chapters 0 through 3, and if time permits, part of chapter 4.

Grading: Your grade will be based on the following –

1. Four tests (including the final) 80% (20% each)
2. Several quizes 20%

Make-up tests: A test may be made up only if I am contacted within 24 hours after the test is given and if the reason for absence is legitimate.

Attendance plolicy: Students are expected to attend class. A student who must miss class is expected to obtain the assignment and be prepared for the next class meeting.

Honor code: All students are expected to abide by the ODU Honor Code. This means that all exams submitted are to be the exclusive work of the student. An honor pledge will be required on all work which is graded.

1.1 Mathematical Models and Reasoning

1.1.1 Hand-Out of Reasoning Problems

1. (a) All Students who major in philosophy wear Calvert Kreem jeans.
   (b) None of the students in the Marching and Chowder Society wears Clavert Kreem jeans or majors in history.
   (c) If Jack majors in philosophy, Mary majors in history.

   Question: If the statements above are all true, which of the following must also be true?

   (A) If Jack majors in philosophy, Mary does not wear Calvert Kreem jeans.
   (B) None of the students in the Marching and Chowder Society majors in philosophy.
   (C) If Jack wears Calvert Kreem jeans, he majors in philosophy.
   (D) If Mary majors in history, Jack is not in the Marching and Chowder Society.
   (E) Either Jack or Mary wears Calvert Kreem jeans.

   Question: The conclusion "Jack does not major in philosophy" could be validly drawn from the statements above if it were established that

   I. Mary does not major in history.
   II. Jack does not belong to the Marching and Chowder Society.
   III. Jack does not wear Calvert Kreem jeans.

   (A) I only, (B) II only, (C) III only, (D) I and III, (E) II and III

2. All good athletes want to win, and all athletes who want to win eat a well-balanced diet; therefore, all athletes who do not eat a well-balanced diet are bad athletes.

   Question: If the argument above is valid, then which of the following statements must be true?

   (A) No bad athlete wants to win.
   (B) No athlete who does not eat a well-balanced diet is a good athlete.
   (C) Every athlete who eats a well-balanced diet is a good athlete.
   (D) All athletes who want to win are good athletes.
   (E) Some good athletes do not eat a well-balanced diet.

   Question: Which of the following, if true, would weaken the argument above?

   (A) Ann wants to win, but she is not a good athlete.
   (B) Bob, the accountant, eats a well-balanced diet, but he is not a good athlete.
   (C) All the players on the Burros baseball team eat a well-balanced diet.
   (D) No athlete who does not eat a well-balanced diet wants to win.
   (E) Cindy, the basketball star, does not eat a well-balanced diet, but she is a good athlete.

1.1.2 Introduction

Mathematical modeling is a model which is an analogy for an object, phenomenon, or process. A mathematical model is a model based on mathematically stated principles. Because of the rigor and lack of ambiguity, it provides a good means for expressing *principles.* It has three components:

1. The phenomena or process that is to be modeled.
2. A math structure which is used to make assertions about the object being modeled.
3. A correspondence between the real world object and the math structure.

Example: Consider the position function $f(t) = 4t^2 + t + 16$ where t represents time and $f(t)$ represents position.

Here is a list of reasons for using models.

1. To present information in a form which is easily understood.
2. To provide a means for simplifying computations.
3. To predict parameter values for events which have not yet occurred.

The value of a model is best measured by its ability to answer questions and to make predictions about the object being modeled.

1.1.3 Mathematical Reasoning

A *proposition* is a statement which is either true or false but not both. We say that the true value of the statement is True or False.

Example: $2 + 4 \leq 3$ is False.

Example: 0 is an integer is True.

Example: $2x = 8$ is not a proposition.

Example: "Close the door" is not a proposition.

Example: "This sentence is false" is not a proposition because it is both True and False.

Notation: We use capital letters beginning with P to denote arbitrary propositions. The following is a list of operations on propositions.

1. Negation or not is denoted by $\neg$. The *truth table* is:

P	$\neg P$
T	F
F	T

   The value True can also be defined as True $\equiv 1$ and the value False can be defined as False $\equiv 0$.

2. Conjunction (i.e. and) is denoted by $\wedge$. The truth table is:

P	Q	$P \wedge Q$
0	0	0
0	1	0
1	0	0
1	1	1

3. Disjunction (i.e. or) is denoted by $\vee$. The truth table is:

P	Q	$P \vee Q$
0	0	0
0	1	1
1	0	1
1	1	1

4. Exclusive Or is denoted by $\oplus$. The truth table is:

P	Q	$P \oplus Q$
0	0	0
0	1	1
1	0	1
1	1	0

5. Implication is denoted by $\Rightarrow$. The truth table is:

P	Q	$P \Rightarrow Q$
0	0	1
0	1	1
1	0	0
1	1	1

$Q \Rightarrow P$ is called the *converse* of $P \Rightarrow Q$.

$\neg Q \Rightarrow \neg P$ is called the *contra-positive* of $P \Rightarrow Q$.

$\neg P \Rightarrow \neg Q$ is called the *inverse* of $P \Rightarrow Q$.

6. Equivalence is denoted by $\Leftrightarrow$. The truth table is:

P	Q	$P \Leftrightarrow Q$
0	0	1
0	1	0
1	0	0
1	1	1

Note that $P \Leftrightarrow Q$ means the same thing as $(P \Rightarrow Q) \wedge (Q \Rightarrow P)$.

P	Q	$P \Rightarrow Q$	$Q \Rightarrow P$	$(P \Rightarrow Q) \wedge (Q \Rightarrow P)$
0	0	1	1	1
0	1	1	0	0
1	0	0	1	0
1	1	1	1	1

Here are some more properties. $(P \vee \neg Q) \Rightarrow \neg P$.

P	Q	$\neg Q$	$P \vee \neg Q$	$\neg P$	$(P \vee \neg Q) \Rightarrow \neg P$
0	0	1	1	1	1
0	1	0	0	1	1
1	0	1	1	0	0
1	1	0	1	0	0

The *distributive property* is $[P \wedge (Q \vee R)] \Leftrightarrow [(P \wedge Q) \vee (P \wedge R)]$.

P	Q	R	$Q \vee R$	$P \wedge (Q \vee R)$	$P \wedge Q$	$P \wedge R$	$(P \wedge Q) \vee (P \wedge R)$
0	0	0	0	0	0	0	0
0	0	1	1	0	0	0	0
0	1	0	1	0	0	0	0
0	1	1	1	0	0	0	0
1	0	0	0	0	0	0	0
1	0	1	1	1	0	1	1
1	1	0	1	1	1	0	1
1	1	1	1	1	1	1	1

A *tautology* is a proposition which is always true. A *contridiction* is a proposition which is always false. A *contigency* is a proposition which is not a tautology and is not a contradiction. It is true part of the time and false part of the time.

Identities on page 15 of the text book. 7, 8, 18, 22. Delete 20 and 21. Logical implications on page 16 of the text book. Delete 7, 8, and 9. For homework, on page 17 in Section 1.1 of the text book, do problems 1, 3, 4, 5, and 7. Also show $(P \Leftrightarrow Q) \Leftrightarrow [(P \Rightarrow Q) \wedge (Q \Rightarrow P)]$.

1.1.4 Homework and Answers

These are the homework problems from Section 1.1 on pages 17 and 18 in the textbook.

Show $(P \Leftrightarrow Q) \Leftrightarrow [(P \Rightarrow Q) \wedge (Q \Rightarrow P)]$.

P	Q	$P \Leftrightarrow Q$	$P \Rightarrow Q$	$Q \Rightarrow P$	$(P \Rightarrow Q) \wedge (Q \Rightarrow P)$
0	0	1	1	1	1
0	1	0	1	0	0
1	0	0	0	1	0
1	1	1	1	1	1

3. Establish whether the following propositions are tautologies, contigencies, or contradictions.

a) $P \vee \neg P$ Tautology.
b) $P \wedge \neg P$ Contridiction.
c) $P \Rightarrow \neg(\neg P)$

P	$P \Rightarrow \neg(\neg P)$
0	0 1
1	1 0

$\Rightarrow$ contingency

d) $\neg(P \wedge Q) \Leftrightarrow (\neg P \vee \neg Q)$. Tautology.

e) $\neg(P \vee Q) \Leftrightarrow (\neg P \wedge \neg Q)$. Tautology.

f) $(P \Rightarrow Q) \Leftrightarrow (\neg Q \Rightarrow \neg P)$. Tautology.

g) $(P \Rightarrow Q) \wedge (Q \Rightarrow P)$.

$(P \Rightarrow Q) \wedge (Q \Rightarrow P)$
0 1 0 1 0 1 0
0 1 1 0 1 0 0
1 0 0 0 0 1 1
1 1 1 1 1 1 1

$\Rightarrow$ contingency

h) $[P \wedge (Q \vee R)] \Rightarrow [(P \wedge Q) \vee (P \wedge R)]$. Tautology.

i) $(P \wedge \neg P) \Rightarrow Q$. Taugology.

j) $(P \vee \neg Q) \Rightarrow Q$.

P	Q	$P \vee \neg Q$	$(P \vee \neg Q) \Rightarrow Q$	
0	0	1	0	
0	1	0	1	$\Rightarrow$ contingency
1	0	1	0	
1	1	1	1	

k) $P \Rightarrow (P \vee Q)$.

P	Q	$P \vee Q$	$(P \Rightarrow (P \vee Q)$	
0	0	0	1	
0	1	1	1	$\Rightarrow$ tautology
1	0	1	1	
1	1	1	1	

l) $(P \wedge Q) \Rightarrow P$.

P	Q	$P \wedge Q$	$(P \wedge Q) \Rightarrow P$	
0	0	0	1	
0	1	0	1	$\Rightarrow$ tautology
1	0	0	1	
1	1	1	1	

m) $(P \wedge Q) \Leftrightarrow P] \Leftrightarrow [P \Leftrightarrow Q]$

P	Q	$P \wedge Q$	$(P \wedge Q) \Leftrightarrow P$	$P \Leftrightarrow Q$	$[(P \wedge Q) \Leftrightarrow P] \Leftrightarrow [P \Leftrightarrow Q]$	
0	0	0	1	1	1	
0	1	0	1	0	0	$\Rightarrow$ contingency
1	0	0	0	0	1	
1	1	1	1	1	1	

n) $[(P \Rightarrow Q) \vee (R \Rightarrow S)] \Rightarrow [(P \vee R) \Rightarrow (Q \vee S)]$.

$$[(\neg P \vee Q) \vee (\neg R \vee S)] \Rightarrow [\neg(P \vee R) \vee (Q \vee S)],$$

$$\neg[(\neg P \vee Q) \vee (\neg R \vee S)] \vee [\neg(P \vee R) \vee (Q \vee S)],$$

$$[\neg(\neg P \vee Q) \wedge \neg(\neg R \vee S)] \vee [(\neg P \wedge \neg R) \vee (Q \vee S)],$$

$$[(P \wedge \neg Q) \wedge (R \wedge \neg S)] \vee [(\neg P \wedge \neg R) \vee (Q \vee S)].$$

Complete the truth table. Contingency.

4. Let P be the proposition "It is snowing." Let Q be the proposition "I will go to town." Let R be the proposition "I have time." Using logical connectives, write a proposition which symbolizes each of the following:

4a. i) If it is not snowing and I have time, then I will go to town. $(\neg P \wedge R) \Rightarrow Q$,

ii) I will go to town only if I have time. $Q \Rightarrow R$.

iii) It isn't snowing. $\neg P$.

iv) It is snowing and I will not go to town. $P \wedge \neg Q$.

4b. i) $Q \Leftrightarrow (R \wedge \neg P)$. I will go to town is equivalent to I have time and it is not snowing.

ii) $R \wedge Q$. I have time, and I will go to town.

iii) $(Q \Rightarrow R) \wedge (R \Rightarrow Q)$. If I will go to town then I have time, and If I have time then I will go to town.

iv) $\neg(R \vee Q)$. I don't have time and I won't go to town.

5. State the converse and contrapositive of each of the following:

a. If it rains, I'm not going. Solution: If I'm not going, it rains. If you don't go then it won't rain.

b. I will stay only if you go. Solution: If you go then I will stay. If you don't go then I won't stay.

c. I you get 4 pounds, you can bake the cake. Solution: If you bake the cake, you get 4 pounds. If you don't bake the cake then you won't get 4 pounds.

d. I can't complete the task if you don't get more help. Solution: If I can't complete the task, then I don't get more help. If I can complete the task, then I get more help.

7. Establish the following tautologies by simplifying the left side to the form of the right side:

a. $[(P \wedge Q) \Rightarrow P] \Leftrightarrow 1$ Solution:
$\neg(P \wedge Q) \vee P$
$(\neg P \vee \neg Q) \vee P$
$(\neg P \vee P) \vee \neg Q$
$1 \vee \neg Q$
1

b. $\neg(\neg(P \vee Q) \Rightarrow \neg P) \Leftrightarrow 0$, Solution:
$\neg((P \vee Q) \vee \neg P)$,
$\neg(P \vee Q) \wedge P$,
$(\neg P \wedge \neg Q) \wedge P$,
$(\neg P \wedge P) \wedge \neg Q$,
$0 \wedge \neg Q$,
0.

1.1.5 Predicates and Quantifiers

Quiz on Section 1.1 on Monday. It will cover truth tables, tautologies, etc. Don't have to know identities.

The statement $P \Leftrightarrow Q$ can be re-stated several ways, such as P if and only if Q or P iff Q.

A *predicate* is a property of an object or a relationship between objects.

Example: $x < y$ means x is less than y where the phrase "is less than y" is the predicate. "x is an integer is an integer" where the phrase "is an integer" is a predicate.

Notation: Assertions made with predicates are denoted with capital letters.

Example: x is less than $y \to L(x, y)$.

Example: x is tall $\to T(x)$.

Example: $x + y = z \to S(x, y, z)$.

The predicate (P) $P(x_1, x_2, ..., x_n)$ is said to have n arguments with individual variables $x_1, x_2, ..., x_n$. Values for the variables are drawn from a non-empty set called the *universe,* denoted by U.

Example: Let $P(x, y)$ mean $x \leq y$ where U is the set of integers. Then, $P(3, 5)$ is True. $P(6, 6)$ is True. $P(6, 2)$ is False.

Example: Let $S(x, y)$ mean $x - y = 5$ and U be the set of integers. Then, $S(12, 7)$ is True. $S(4, -2)$ is False.

To change a predicate into a proposition, each individual variable must be *bound.* There are two ways to do this:

1. A variable is bound when a value is assigned to it.
2. A variable is bound when it is *quantified.*

This is a list of quantifiers:

1. The universal quantifier $\forall$ (for all). $\forall x\ P(x)$ means for all x, $P(x)$ is true if the predicate $P(x)$ is true for all x in the universe. Otherwise, $\forall x\ P(x)$ is false.

   Example: Let U be the set of integers. $\forall x\ [x > 0]$ is False.

   Example: Let U be the set of natural numbers $\{1, 2, 3...\}$. $\forall x\ [x > 0]$ is True.

   Example: Let U be the set of integers. $\forall x \forall y\ [x + y > x]$ is False.

   Example: Let U be the set of integers. $\forall x \forall y\ [2(x + y) = 2x + 2y]$ is True.

   Note that $\forall x\ P(x) \Rightarrow P(c)$ is true for any c in the universal set. The notation $\{c \in U\}$ is also used.

2. The existential quantifier $\exists$ (there exists or for some). $\exists x\ P(x)$ means there exists x such that $P(x)$ is true if $P(x)$ is true for at least one $x \in U$, otherwise $\exists x\ P(x)$ is false.

   Example: Let U be the set of integers. $\exists x\ [x > 2]$ is true.

   Example: Let U be the set of natural numbers. $\exists x\ [x = 0]$ is false.

   Note that if $P(c)$ is true, then $\exists x\ P(x)$ is true.

3. The unique existential quantifier $\exists!$ (one and only one). $\exists! x\ P(x)$ is true if $P(x)$ is true for exactly one element in U.

   Example: Let U be the set of natural numbers. $\exists! x\ [x < 1]$ is false.

Example: Let U be the set of natural numbers. $\exists! x\ [x = 3]$ is true.

Example: Let U be the set of natural numbers. $\exists! x\ [x < 2]$ is true.

Note: Let $P(x)$ represent $x \leq 5$ where U is the set of natural numbers. Then, $\forall x\ P(x) = P(1) \wedge P(2) \wedge P(3) \wedge P(5) \wedge P(6) \cdots$.

In general, $\forall x\ P(x) = P(x_0) \wedge P(x_1) \wedge \cdots$.

all	at least one	uniqueness
$\forall x\ P(x)$	$\exists x\ P(x)$	$\exists! x\ P(x)$
$\wedge$	$\vee$	$P(x_0) \oplus P(x_1) \oplus P(x_2) \cdots$

When combining more than one quantifier, order is important in predicates with more than one quantifier. The notation $\forall x \forall y\ P(x, y)$ means $\forall x [\forall y\ P(x, y)]$.

Example: $\forall x [\exists y\ P(x, y)]$: for every x there is some y — not necessarilary the same y.

Example: $\exists y [\forall x\ P(x, y)]$: there is some y such that for every x there is a value which makes P true.

Example: $\forall x \forall y\ P(x, y) = \forall y \forall x\ P(x, y)$.

Example: $\exists x \exists y\ P(x, y) = \exists y \exists x\ P(x, y)$.

Read the examples on page 26 in the text book. In Section 1.2 on page 27, do problems 1, 3, 5(d*), 7, and 9.

1.1.6 Quiz 1

1. Using truth tables, show that an implication is equivalent to its contrapositive. Solution:

P	Q	$P \Rightarrow Q$	$\neg Q$	$\neg P$	$\neg Q \Rightarrow \neg P$	$P \Rightarrow Q \Leftrightarrow \neg Q \Rightarrow \neg P)$
0	0	1	1	1	1	1
0	1	1	0	1	1	1
1	0	0	1	0	0	1
1	1	1	0	0	1	1

2. Make a truth table for $(\neg Q \wedge P) \vee (\neg P \Rightarrow Q)$. Is this proposition a tautology, contingency, or contradiction? Solution: contingency.

P	Q	$\neg Q$	$\neg Q \wedge P$	$\neg P$	$\neg P \Rightarrow Q$	$(\neg Q \wedge P) \vee (\neg P \Rightarrow Q)$
0	0	1	0	1	0	0
0	1	0	0	1	1	1
1	0	1	1	0	1	1
1	1	0	0	0	1	1

3. Le P : dogs bark. Q : cats bite. R : horses swim. Write each of the following in symbolic form.

   (a) Horses swim if and only if cats do not bite. Solution: $R \Leftrightarrow \neg Q$.

   (b) If horses swim then dogs do not bark, and if dogs do not bark then cats bite. Solution: $(R \rightarrow \neg P) \wedge (\neg P \Rightarrow Q)$.

   (c) Either dogs bark or cats bite, but not both. Solution: $(P \vee Q) \wedge \neg (P \wedge Q)$.

   (d) It is not the case that horses do not swim and dogs do not bark. Solution: $\neg(\neg R \wedge \neg P)$.

1.1.7 Quantifiers with Negation

This section covers quantifiers with negation.

1. $\neg\forall x\ P(x)$ means $\exists x \neg\ P(x)$. Proof:

$$\neg(P(x_0) \wedge P(x_1) \wedge P(x_2) \wedge \cdots) =$$

$$\neg P(x_0) \vee \neg P(x_1) \vee \neg P(x_2) \vee \cdots =$$

$$\exists x \neg\ P(x).$$

$\neg\exists x\ P(x)$ means $\forall x\ \neg P(x)$. Proof:

$$\neg(P(x_0) \vee P(x_1) \vee P(x_2) \vee \cdots) =$$

$$\neg P(x_0) \wedge \neg P(x_1) \wedge \neg P(x_2) \wedge \cdots =$$

$$\forall x \neg P(x).$$

$\neg\forall x \exists y \forall z\ P(x, y, z) = \exists x \forall y \exists z \neg P(x, y, z).$

2. Conjunction: $\forall x[P(x) \wedge Q(x)] \Leftrightarrow \forall x\ P(x) \wedge \forall x\ Q(x)$. Proof:

$$[P(x_0) \wedge Q(x_0)] \wedge [P(x_1) \wedge Q(x_1)] \wedge [P(x_2) \wedge Q(x_2)] \wedge \cdots$$

Regroup.

$$[P(x_0) \wedge P(x_1) \wedge P(x_2) \wedge \cdots] \wedge [Q(x_0) \wedge Q(x_1) \wedge Q(x_2) \wedge \cdots] =$$

$$\forall x\ P(x) \wedge \forall x\ Q(x).$$

Here are some properties:

1. $\neg\forall x\ P(x) \Leftrightarrow \exists x\ \neg P(x)$.
2. $\neg\exists x\ P(x) \Leftrightarrow \forall x\ \neg P(x)$.
3. $\forall x P(x) \wedge Q(x)) \Leftrightarrow \forall x\ P(x) \wedge \forall x\ Q(x)$. This is not the same as $\exists x(P(x) \wedge Q(x)) \neq \exists x\ P(x) \wedge \exists x\ Q(x)$. Left-proof:

$$(P(x_0) \wedge Q(x_0)) \vee (P(x_1) \wedge Q(x_1)) \vee (P(x_2) \wedge Q(x_2)) \vee \cdots.$$

$$\exists x\ P(x) \wedge \exists x\ Q(x) \Leftrightarrow$$

Right-proof:

$$[P(x_0) \vee P(x_1) \vee P(x_2) \vee \cdots] \wedge [Q(x_0) \vee Q(x_1) \vee Q(x_2) \vee \cdots].$$

4. $\exists x(P(x) \wedge Q(x)) \Rightarrow \exists x\ P(x) \wedge \exists x\ Q(x)$ is true.
5. $\forall x(P(x) \vee Q(x)) \not\Rightarrow \forall x\ P(x) \vee \forall x\ Q(x)$. Also, $\exists x(P(x) \vee Q(x)) \Leftrightarrow \exists x\ P(x) \vee \exists x\ Q(x)$.
6. $\forall x(P(x) \vee Q(x)) \Leftarrow \forall x\ P(x) \vee \forall x\ Q(x)$.

The *scope* of a quantifier is that part of an assertion in which variables are bound by the quantifier. It is the smallest subexpression which is consistent with the parenthesis of the expression.

Example: $\forall x[P(x) \wedge Q]$. The scope of $\forall$ is $[P(x) \wedge Q]$.

Example: $\forall x P(x) \wedge Q$. The scope of $\forall$ is $P(x)$.

Example: $\forall x P(x) \wedge Q(x) \Leftrightarrow \forall y P(y) \wedge Q(x)$. The scope of $\forall$ is $P(x)$.

Result: Predicates which occur in $\vee$ and $\wedge$ assertions and which are not bound by a quantifier may be removed from the scope of the quantifier.

Example: $\forall x[P(x) \wedge Q] \Leftrightarrow \forall x\ P(x) \wedge Q$. Q is not bound by $\forall$. Proof:

$$\forall x[P(x) \wedge Q] \Leftrightarrow$$

$$[P(x_0) \wedge Q] \wedge [P(x_1) \wedge Q] \wedge [P(x_2) \wedge Q] \wedge \cdots$$

$$[P(x_0) \wedge P(x_1) \wedge P(x_2) \wedge \cdots] \wedge [Q \wedge Q \wedge Q \wedge \cdots]$$

$$\forall x\ P(x) \wedge Q.$$

Example: $\forall x[P(x) \wedge Q] \Leftrightarrow \forall x\ P(x) \vee Q$. Proof:

$$[P(x_0) \vee Q] \wedge [P(x_1) \vee Q] \wedge [P(x_2) \vee Q] \wedge \cdots$$

$$[P(x_0) \wedge P(x_1) \wedge P(x_2) \wedge \cdots] \vee Q$$

$$\forall x\ P(x) \vee Q.$$

Example: $\exists x[P(x) \wedge Q] \Leftrightarrow \exists x\ P(x) \wedge Q$.

Example: $\exists x[P(x) \vee Q] \Leftrightarrow \exists x\ P(x) \vee Q$.

Example: $\forall x[P(x) \wedge Q(y)] \Leftrightarrow \forall x\ P(x) \wedge Q(y)$.

In Section 1.3 of the textbook, page 37, do problems 1a-d, 2, 3a-c, 4, 9. On Friday, Quiz 2 which will cover Sections 1.2 and 1.3.

1.1.8 Homework and Answers

Section 1.2 homework and answers on Page 27 of the textbook.

1. Let $S(x,y,z)$ denote the predicate $x+y-z$, $P(x,y,z)$ denote $x \cdot y = z$, and $L(x,y)$ denote $x < y$. Let the universe of discourse be the natural numbers N. Using the above predicates, express the following assertions. The phrase "there is an x" does not imply that x has a unique value.

a. For every x and y, there is a z such that $x+y=z$. Solution: $\forall x \forall y \ S(x,y,z)$.

b. No x is less than 0. Solution: $\forall x \neg L(x,0)$.

c. For all x, $x+0=x$. Solution: $\forall x \ S(x,0,0)$.

d. For all x, $x \cdot y = y$ for all y. Solution: $\forall x \forall y \ P(x,y,y)$.

e. There is an x such that $x \cdot y = y$ for all y. Solution: $\exists x \forall y \ P(x,y,y)$.

3. Determine which of the following propositions are true if the universe is the set of integers I and $\cdot$ denotes the operation of multiplication.

a. $\forall x, \exists y[x \cdot y = 0]$. True

b. $\forall x, \exists ! y[x \cdot y = 1]$. False $(x=0)$.

c. $\exists y, \forall x[x \cdot y = 1]$. False.

d. $\exists y, \forall x[x \cdot y = x]$. True.

5. Specify a universe discourse for which the following propositions are true. Try to choose the universe to be as large a subset of the integers as possible. Explain any difficulties.

a. $\forall x[x > 10]$. Solution: $U = \{11, 12, 13, ...\}$.

b. $\forall x[x = 3]$. Solution: $U = \{3\}$.

c. $\forall x \exists y[x+y=436]$. Solution: $U =$ integers.

d. $\exists y \forall x[x+y<0]$. Solution: $U =$ integers, $|y| > |x|$.

7. Consider the univers of integers I.

a. Find the predicate $P(x)$ which is false regardless of whether the variable x is bound by $\forall$ or $\exists$. Solution: $x = x+1$. $P(x)[x = \frac{1}{2}]$.

b. Find the predicate $P(x)$ which is true regardless of whether the variable x is bound by $\forall$ or $\exists$. Solution: $x = x$. $[x+1 > x]$.

c. Is it possible for a predicate $P(x)$ to be true regardless of whether the variable is bound by $\forall, \exists$ or $\exists !$? Justify your answer. Solution: Yes. The universal set equal to one element say 1 [$x=1$ for all cases].

9. Consider the universe of integers and let $P(x,y,z)$ denote $x-y=z$. Transcribe the following assertions into logical notation.

a. For every x and y, there is some z such that $x-y=z$. Solution: $\forall x \forall y \exists z \ P(x,y,z)$.

b. For every x and y, there is some z such that $x-z=y$. Solution: $\forall x \forall z \exists y \ P(x,y,z)$.

c. There is an x such that for all y, $y-x=y$. Solution: $\exists x \forall y \ P(x,y,y)$.

d. When 0 is subtracted from any integer, the result is the original integer. Solution: $\forall x \exists y \ P(x,y,x)$.

e. 3 subtracted from 5 gives 2. Solution: $P(5,3,2)$.

Some additional observations: If $\exists P(x)$ is false, then $\forall x \ P(x)$ is false. If $\forall x \ P(x)$ is true, then $\exists x \ P(x)$ is true.

1.1.9 Homework and Answers

This is Section 1.3 homework and answers on page 37 from the textbook.

1. Let $P(x, y, z)$ denote $xy = z$. Let $E(x, y)$ denote $x = y$. Let $G(x, y)$ denote $x > y$. Let the universe of discourse be the integers. Transcribe the following into logical notation.

a. If $y = 1$, then $xy = x$ for any x. Solution: $\forall y[E(y, 1) \Rightarrow \forall x \; P(x, y, x)]$.

b. If $xy \neq 0$, then $x \neq 0$ and $y \neq 0$. Solution: $\forall x\forall y[\neg P(x, y, 0) \Rightarrow \neg E(x, 0) \wedge \neg E(y, 0)]$.

c. If $xy = 0$, then $x = 0$ or $y = 0$. Solution: $\forall x\forall y[P(x, y, 0) \Rightarrow E(x, 0) \vee E(y, 0)]$.

d. $3x = 6$ if and only if $x = 2$. Solution: $\forall x[P(3, x, 6) \Leftrightarrow E(x, 2)]$.

2. Let the universe of discourse be the set of arithmetic assertions with predicates defined as follows: $P(x)$ denotes "x is provable. $T(x)$ denotes "x is true." $S(x)$ denotes "x is satisfiable." $D(x, y, z)$ denotes "z is the disjuntion $x \vee y$." Translate the following assertions into English statements. Make your transcriptions as natural as possible.

a. $\forall x[P(x) \Rightarrow T(x)]$. Solution: For all arithmetic assertions x such that if x is provable, then x is true.

b. $\forall x[T(x) \vee \neg S(x)]$. Solution: For all x such that x is true or x is not satisiable.

c. $\exists x[T(x) \wedge \neg P(x)]$. Solution: For all x such that if x is true, then x is not provable.

d. $\forall x\forall y\forall z[[D(x, y, z) \wedge P(z)] \Rightarrow [P(x) \vee P(y)]]$. Solution: For all x, y, and z if z is disjunction $x \vee y$ and z is provable, then x is provable or y is provable.

e. $\forall x[T(x) \Rightarrow \forall y\forall z[D(x, y, z) \Rightarrow T(z)]]$. Solution: For all x if x is true, then for all y and z if z is the disjunction $x \vee y$ then z is true.

3. Put the following into logical notation. Choose predicates so that each assertion requires at least one quantifier.

a. There is one and only one even prime. Solution: $P(x) =$ the even numbers. $Q(x) =$ the prime numbers. $\exists! x \; [P(x) \wedge Q(x)]$.

b. No odd numbers are even. Solution: $P(x) =$ the even numbers. $Q(x) =$ the odd numbers. $\forall x \; [Q(x) \Rightarrow \neg P(x)]$. $\forall x[\neg P(x) \vee \neg Q(x)]$.

c. Every train is faster than some cars. Solution: $P(x) =$ trains. $Q(y) =$ cars. $R(x, y) =$ trains travel faster than cars. $\forall x[P(x) \Rightarrow \exists y[Q(y) \wedge R(x, y)]$.

d. Some cars are slower than all trains but at least one train is faster than every car. Solution: $\exists x \neg P(x)$. $\neg\forall x \; P(x)$.

9. Show that the following are valid for the universe of natural numbers N either by expanding the statement or by applying identities.

a. $\forall x\forall y[P(x) \vee Q(y)] \Leftrightarrow [\forall x P(x) \vee \forall y Q(y)]$. Solution: $\forall x\forall y[P(x) \vee Q(y)] \Leftrightarrow [\forall x \; P(x) \vee \forall y \; Q(y)]$.

$$\forall x[\forall y[P(x) \vee Q(y)] \Leftrightarrow$$

$$\forall x[P(x) \vee \forall y Q(y)] \Leftrightarrow$$

$$\forall x P(x) \vee \forall y Q(y).$$

b. $\exists x \exists y[P(x) \wedge Q(y)] \Rightarrow \exists x P(x)$. Solution: $P \wedge Q \Rightarrow P$.

e. $\forall x \forall y[P(x) \Rightarrow Q(y)] \Leftrightarrow [\exists x P(x) \Rightarrow \forall y Q(y)]$. Solution:

$$\forall x \forall y[P(x) \Rightarrow Q(y)] \Leftrightarrow$$

$$\forall x \forall y[\neg P(x) \vee Q(y)]$$

$$\forall x \neg P(x) \vee \forall y Q(y)$$

$$\neg \exists x P(x) \vee \forall y Q(y)$$

$$\exists x P(x) \Rightarrow \forall y Q(y).$$

1.1.10 Quiz 2

September 11, 1987

1. Let the universe be the set of integers. Determine whether each of the following propositions is True or False. Explain your answers.

   (a) $\forall x \exists ! y[3x - y = 5]$. Solution: True because if x is positive, y can be negative. If x is negative, y can be positive to make up the difference.

   (b) $\exists x[x = \frac{1}{x}]$. Solution: True at $x = 1$. $\exists$ only takes at least one case to make it true.

   (c) $\forall x \exists y[x = 2y]$. Solution: False. What if x is an odd number? Then, y would have to be a real number that is not in the universe.

   (d) $\forall x \forall y[(x + y > 0) \vee (x + y < 0)]$. Solution: False. What if x and y equal to zero? Then neither case would hold true.

   (e) $\exists y \forall x[y \cdot x = x]$. Solution: True for the case $y = 1$. Then, any x would hold true.

2. Prove the following identity by expanding the left-hand side. $\forall x \neg P(x) \Leftrightarrow \neg \exists x P(x)$. Solution:
   $\neg P(x_0) \wedge \neg P(x_1) \wedge \neg P(x_2) \wedge \cdots \Leftrightarrow$
   $\neg(P(x_0) \vee P(x_1) \vee P(x_2) \vee \cdots) \Leftrightarrow$
   $\neg \exists x P(x)$.

3. Prove the following identity by expanding the left-hand side. $\exists x[Q(y) \wedge P(x)] \Leftrightarrow Q(y) \wedge \exists x P(x)$. Solution:
   $(Q(y) \wedge P(x_0)) \vee (Q(y) \wedge P(x_1)) \vee (Q(y) \wedge P(x_2)) \vee \cdots) \Leftrightarrow$
   $Q(y) \wedge (P(x_0) \vee P(x_1) \vee P(x_2) \vee \cdots) \Leftrightarrow$
   $Q(y) \wedge \exists x P(x)$

1.1.11 Logical Inferences

A *proof* is a sequence of statements which establishes that a theorem is true. The sequence of assertions in a proof consists of three things:

1. Axioms or previously proved theorems.
2. Hypotheses of the theorem.
3. Assertions inferred from previous assertions in the proof.

Some rules of inference include:

1. Modus ponens

$$\begin{array}{l} P \\ P \Rightarrow Q \\ \hline \therefore Q \end{array}$$

Example:

$$\begin{array}{l} \text{If it rains, then I will study.} \\ \text{It rains.} \\ \hline \therefore \text{ I will study.} \end{array}$$

An argument iff, the conjunction of the hypotheses, implies the conclusion is a tautology.

P	Q	$P \Rightarrow Q$	$P \wedge (P \Rightarrow Q)$	$[P \wedge (P \Rightarrow Q)] \Rightarrow Q$
0	0	1	0	1
0	1	1	0	1
1	0	0	0	1
1	1	1	1	1

2. Modus tollens.

$$\begin{array}{l} \neg Q \\ P \Rightarrow Q \\ \hline \therefore \neg P \end{array}$$

3. Addition.

$$\begin{array}{l} P \\ \hline \therefore P \vee Q \end{array}$$

4. Simplification.

$$\begin{array}{l} P \wedge Q \\ \hline \therefore P \end{array}$$

5. Disjunctive syllogism.

$$\begin{array}{l} P \vee Q \\ \neg P \\ \hline \therefore Q \end{array}$$

$[(P \vee Q) \wedge \neg P] \Rightarrow Q$.

6. Hypothetical syllogism.

$$\begin{array}{l} P \Rightarrow Q \\ Q \Rightarrow R \\ \hline \therefore P \Rightarrow R \end{array}$$

7. Conjunction.

$$\begin{array}{l} P \\ Q \\ \hline \therefore P \wedge Q \end{array}$$

8. Constructive delimma.

$$\begin{array}{l} (P \Rightarrow Q) \wedge (R \Rightarrow S) \\ P \vee R \\ \hline \therefore Q \vee S \end{array}$$

9. Destructive delimma.

$$\begin{array}{l} (P \Rightarrow Q) \wedge (R \Rightarrow S) \\ \neg Q \vee \neg S \\ \hline \therefore \neg P \vee \neg R \end{array}$$

Some fallacious agruments include the following:

$$\begin{array}{l} P \Rightarrow Q \\ Q \\ \hline \therefore P \end{array}$$

and

$$\begin{array}{l} P \Rightarrow Q \\ \neg P \\ \hline \therefore \neg Q \end{array}$$

Some more complex arguments:

Example: Prove that the following argument is valid.

$$\begin{array}{l} 1. P \Rightarrow Q \\ 2. Q \Rightarrow R \\ 3. \neg R \\ \hline \therefore \neg P \end{array}$$

	Assertions	Reasons
1.	$P \Rightarrow Q$	Hypothesis 1
2.	$Q \Rightarrow R$	Hypothesis 2
3.	$P \Rightarrow R$	Hypotheses 1,2 and hypothetical syllogism
4.	$\neg R$	Hypothesis 3
5.	$\neg P$	Hypotheses 3,4 and modus tollens

Exam #1 will be on Monday, September 21. It covers Sections 1.1 thru 1.4.

Example:

$$\begin{array}{l} 1.R \Rightarrow \neg S \\ 2.\neg M \Rightarrow T \\ 3.\neg P \Rightarrow R \\ 4.T \Rightarrow S \\ \hline \therefore \neg P \Rightarrow M \end{array}$$

	Assertions	Reasons
1.	$\neg P \Rightarrow R$	Hypothesis 3
2.	$R \Rightarrow \neg S$	Hypothesis 1
3.	$\neg S \Rightarrow \neg T$	Contrapositive
4.	$\neg T \Rightarrow M$	Contrapositive of hypothesis 2
5.	$\neg P \Rightarrow M$	Hypothesis 1,23,4 and hypothetical syllogism

Example: Premises:

$$\begin{array}{l} 1.A \Rightarrow \neg B \\ 2.\neg C \Rightarrow F \\ 3.A \vee \neg C \\ 4.\neg B \Rightarrow D \\ 5.F \Rightarrow H \\ \hline \therefore D \vee H \end{array}$$

	Assertions	Reasons
1.	$A \Rightarrow \neg B$	Hypothesis 1
2.	$\neg B \Rightarrow D$	Hypothesis 4
3.	$A \Rightarrow D$	Hypothesis 1,2
4.	$\neg C \Rightarrow F$	Hypothetical syllogism
5.	$F \Rightarrow H$	Hypotheses 2,5
6.	$\neg C \Rightarrow H$	Hypotheses 4,5 and chain rule
7.	$(A \Rightarrow D) \wedge (\neg C \Rightarrow H)$	Hypotheses 3,6 and conjunction
8.	$A \vee \neg C$	Hypothesis 3
9.	$D \vee H$	Hypotheses 7,8 and constructive delimma

The test covers Sections 1.1 to 1.4, truth tables, the operators $+, -, \oplus, \Rightarrow$, and $\Leftrightarrow$. You must know how to read symbolic form to English and vise-versa; page 15 Table of Identities (omit 20 and 21); page 16 implications (omit 7, 8, and 9); qualifiers — read, figure true / false of propositions; properties; proofs of valid arguments with truth tables; rules of inference (page 41).

1.1.12 Handout

3.

$$\begin{array}{ll} S \Rightarrow L & \text{SON} \Rightarrow \neg L \\ \neg S \Rightarrow \neg F & \neg L \Rightarrow \neg S \\ \text{SON} \Rightarrow \neg L & \neg S \Rightarrow \neg F \\ \hline \therefore & \therefore \text{SON} \Rightarrow \neg F \end{array}$$

4.

$$\begin{array}{l} D \Rightarrow \neg W \\ O \Rightarrow W \\ P \Rightarrow D \end{array} \qquad \begin{array}{l} P \Rightarrow D \\ D \Rightarrow \neg W \\ \neg W \Rightarrow \neg O \\ \hline \therefore p \rightarrow \neg O \end{array}$$

5.

$B \Rightarrow I$	$B \Rightarrow I$
$C \Rightarrow \neg D$	$I \Rightarrow \neg D$
$I \Rightarrow D$	$D \Rightarrow \neg C$
$\therefore$	$\therefore B \Rightarrow \neg C$

1.1.13 Homework Handout Questions and Answers

Verify that the following argument forms are valid.

1. Form:

$$\begin{array}{l} \neg Q \Rightarrow \neg R \\ R \\ P \Rightarrow \neg Q \\ \hline \therefore \neg P \end{array}$$

Solution:

	Assertions	Reasons
1.	$\neg Q \Rightarrow \neg R$	Hypothesis 1
2.	$R \Rightarrow Q$	Assertions 1, Contrapositive
3.	R	Hypothesis 2
4.	$Q \Rightarrow \neg P$	Hypothesis 3, Contrapositive
5.	Q	Assertions 3, 2, Modus ponens
6.	$\neg P$	Assertions 4, 5, Modus ponens

2. Form:

$$\begin{array}{l} (P \Rightarrow \neg Q) \wedge (\neg R \Rightarrow S) \\ \neg P \Rightarrow \neg R \\ \hline \therefore \neg Q \vee S \end{array}$$

Solution:

	Assertions	Reasons
1.	$\neg P \Rightarrow \neg R$	Hypothesis 2
2.	$P \vee \neg R$	Equivalence
3.	$(P \Rightarrow \neg Q) \wedge (\neg R \Rightarrow S)$	Hypothesis 1
4.	$\neg Q \vee S$	Assertions 2,3, Constructive dilemma

3. Form:

$$\begin{array}{l} \neg B \Rightarrow F \\ I \Rightarrow \neg C \\ A \Rightarrow \neg B \\ F \Rightarrow I \\ \hline \therefore A \Rightarrow \neg C \end{array}$$

Solution:

	Assertions	Reasons
1.	$A \Rightarrow \neg B$	Hypothesis 3
2.	$\neg B \Rightarrow F$	Hypothesis 1
3.	$F \Rightarrow I$	Hypothesis 4
4.	$I \Rightarrow \neg C$	Hypothesis 2
5.	$A \Rightarrow \neg C$	Assertions 1,2,3,4, Hypothetical syllogism

4. Form:

$$\begin{array}{l} N \Rightarrow \neg R \\ \neg M \Rightarrow N \\ R \\ P \\ \hline \therefore M \wedge P \end{array}$$

Solution:

	Assertions	Reasons
1.	$N \Rightarrow \neg R$	Hypothesis 1
2.	$R \Rightarrow \neg N$	Hypothesis 1, Contrapositive
3.	$\neg M \Rightarrow N$	Hypothesis 2
4.	$\neg N \Rightarrow M$	Assertion 3, Contrapositive
5.	$R \Rightarrow M$	Assertions 2,4, Hypothetical syllogism
6.	R	Hypothesis 3
7.	M	Assertion 5, 6, Modus ponens
8.	P	Hypothesis 4
9.	$M \wedge P$	Assertion 7, 8, Conjunction

5. Form:

$$\begin{array}{l} \neg F \Rightarrow C \\ \neg C \vee \neg D \\ B \Rightarrow \neg F \\ D \\ \hline \therefore \neg B \end{array}$$

Solution:

	Assertions	Reasons
1.	$\neg C \Rightarrow \neg D$	Hypothesis 2
2.	$C \Rightarrow \neg D$	Hypothesis 2, Equivalence
3.	$D \Rightarrow \neg C$	Assertion 2, Contrapositive
4.	$\neg C \Rightarrow F$	Hypothesis 1, Contrapositive
5.	$F \Rightarrow \neg B$	Hypothesis 3, Contrapositive
6.	D	Hypothesis 4
7.	$\neg B$	Assertions 3, 4, 5, 6, Hypothetical syllogism

1.1.14 Exam 1

1.1.15 Methods of Proof

There are several techniques for proving implications.

1. Vacuous proof of $P \Rightarrow Q$. (Rows 1, 2) Recall $P \Rightarrow Q$ is *True* whenever P is *False.* If we can establish that P is *False,* then we say vacously that $P \Rightarrow Q$ is *True.*

2. Trivial proof of $P \Rightarrow Q$ (Rows 2,4) Observe that $P \Rightarrow Q$ is true whenever Q is *True.* So, if we establish Q as *True,* then $P \Rightarrow Q$ is *True.*

3. Direct proof of $P \Rightarrow Q$. $P \Rightarrow Q$ is *True* when P and Q are both *True.* Assume that P is *True* and show that Q is also *True.*

4. Indirect proof of $P \Rightarrow Q$. We show that the contrapositive is true by direct proof. Assume $\neg Q$ is *True* and show that $\neg P$ is also True.

5. If the premise is a conjunction $(P_0 \wedge P_1 \wedge P_2 \wedge P_3 \cdots \wedge P_n) \Rightarrow Q$, we look at the contrapositive $\neg Q \Rightarrow \neg(P_1 \wedge P_2 \wedge P_3 \wedge \cdots P_n)$ or $\neg Q \Rightarrow \neg P_1 \vee \neg P_2 \vee \neg P_3 \vee \cdots \neg P_n$ is *True* if $\neg Q \Rightarrow \neg P_i$ for at least one i.

6. If the premise is a disjunction,

$$(P_0 \vee P_2 \vee P_3 \vee \cdots \vee P_n) \Rightarrow Q \Leftrightarrow$$

$$\neg(P_0 \vee P_2 \vee P_3 \vee \cdots \vee P_n) \vee Q \Leftrightarrow$$

$$(\neg P_0 \wedge \neg P_2 \wedge \neg P_3 \wedge \cdots \wedge \neg P_n) \vee Q \Leftrightarrow$$

$$(\neg P_0 \vee Q) \wedge (\neg P_2 \vee Q) \wedge (\neg P_3 \vee Q) \wedge \cdots \wedge (\neg P_n \vee Q) \Leftrightarrow$$

$$(P_0 \Rightarrow Q) \wedge (P_2 \Rightarrow Q) \wedge \cdots \wedge (P_n \Rightarrow Q)$$

   is *True* when $P_i \Rightarrow Q$ for all i between 0 and n called a *proof by cases.*

Some other proof techniques include:

1. Proofs of equivalence.
   (a) Use $P \Leftrightarrow Q$ means $(P \Rightarrow Q)$ and $(Q \Rightarrow P)$. Show the two parts seperately. $P \Leftrightarrow Q$ is also read if and only if.
   (b) Begin with an equivalence $R \Leftrightarrow S$ and proceed through a sequence of equivalencies to eventually generate $P \Leftrightarrow Q$.

2. Proof by contradiction. Assume that the opposite with negation is true. Eventually, you arrive at a contridiction. The contradiction implies that the assumption was incorrect.
   Note: Theorem: $P \Rightarrow Q$. Assume $\neg(P \Rightarrow Q)$ is true. Then,

$$\neg(P \Rightarrow Q)$$

$$\neg(\neg P \vee Q)$$

$$(P \wedge \neg Q)$$

   i.e. assume *True* so that P is *True* and Q is *False.* $0 = 1$ is a contradiction to $\neg(P \Rightarrow Q)$ $\therefore P \Rightarrow Q$.

Theorem: For all integers x, x is even iff x^2 is even. Proof: Case 1 (the only if part). Show if x is even, then x^2 is even. $x^2 = (2k)^2 = 4k^2 = 2(2k^2)$ where $2k^2 \in I$. So, x^2 is even. Case 2 (the if part). Show if x^2 is even, then x is even. Use an indirect proof. Prove if x is not even, then x^2 is not even. x is not even $\Rightarrow x$ is odd $\Rightarrow x = 2k+1$ where $k \in I \Rightarrow x^2 = (2k+1)^2 \Rightarrow x^2 = 4k^2 + 4k + 1 \Rightarrow x^2 = 2(2k^2 + 2k) + 1 \in I \therefore x^2$ is odd (i.e. x^2 is not even).

Theorem: If the product of two integers (A and B) is even, then either A is even or B is even. $A \times B$ even $\Rightarrow A$ even $\vee B$ even. Proof (indirect proof):

$$\neg(A \text{ even } \vee B \text{ even }) \Rightarrow \neg AB \text{ even}$$

Show

$$A \text{ odd } \wedge B \text{ odd } \Rightarrow AB \text{ odd}$$

$$A \text{ odd } \wedge B \text{ odd } \Rightarrow A = 2k+1 \wedge B = 2n+1 \;\; k, n \in I$$

$$\Rightarrow AB = (2k+1)(2n+1)$$

$$\Rightarrow AB = 4kn + 2k + 2n + 1 =$$

$$2(2kn + k + n) + 1,$$

$$2kn + k + n \in I$$

$$\therefore AB \text{ is odd.}$$

Theorem: If A is an integer, such that $A-2$ is divisible by 3, then $A^2 - 1 = (A+1)(A-1)$ is divisible by 3. Proof (direct proof): Assume that $A-2$ is divisible by $3 \Rightarrow A-2 = 3k$ where $k \in I \Rightarrow A-2+3 = 3k+3$ $\Rightarrow A+1 = 3(k+1) \Rightarrow A^2 - 1 = (A+1)(A-1) = 3(k+1)(k-1)$. $(k+1), (k-1) \in I \therefore A^2 - 1$ is divisible by 3.

Theorem: If n is a prime number different from 2, then n is odd. A prime number is any natural number greater than 1 which is divisible only by itself and 1.

Proof: By contradiction. Recall that to prove $P \Rightarrow Q$, assume $\neg(P \Rightarrow Q) \Leftrightarrow (P \wedge \neg Q)$. Assume n is prime and $n \neq 2$ and n is even.
n is even
$\Rightarrow n = 2k$ where $k \in$ Interger, $k \neq 1$.
$\Rightarrow n$ is divisible by 2
n is not prime
Contradiction: n is prime.
$\therefore$ If n is prime and $\neq 2$, then n is odd.

Homework: page 56, 1a, b, c, i, j, m.

1.1.16 Proof Techniques for Quantified Assertions

1. Assertions of the form $\neg \exists x P(x)$ can be proved best by contradiction. Assume $\exists x P(x)$ and derive a contradiction.

2. To prove $\exists x P(x)$:

   (a) Constructive existence proof — find a c such that $P(c)$ is true $\Rightarrow \exists x P(x)$ is true.

   (b) Non-constructive existence proof — a proof by contradiction. Assume $\neg \exists x P(x)$ and derive a contradiction.

3. To prove $\neg\forall x P(x)$:

   (a) Constructive proof: Find a particular value of x, c such that $P(c)$ is false.

   (b) Non-constructive proof: proof by contradiction.

4. To prove $\forall x P(x)$ show that $P(x)$ is true for an arbitrary x.

Homework: all of # 1 on page 56 in the textbook.

1.1.17 Homework and Answers

Problem 1 on page 56 in the textbook.

1. Prove or disprove each of the following assertions. Indicate the proof technique employed. Consider the universe to be the the set of integers I. Put each assertion into logical notation. You must assume the following five definitions and properties of itegers.

   1. An integer n is even if and only if $n = 2k$ for some integer k.
   2. An integer n is odd if and only if $n = 2k + 1$ for some integer k.
   3. The product of two non-zero integers is positive if and only if the integers have the same sign.
   4. For every pair of integers x and y, exactly one of the following holds: $x > y$, $x = y$ or $x < y$.
   5. If $x > y$, then $x - y$ is positive. If $x = y$ then $x - y = 0$. If $x < y$, then $x - y$ is negative.

a. An integer is odd if its square is odd. Solution: $\forall x[x^2 \text{ odd} \Rightarrow x \text{ odd}]$. If x^2 is odd, then x is odd. Proof (indirect): If x is not odd, then x^2 is not odd.

   x is not odd $\Rightarrow x$ is even.
   $\Rightarrow x = 2k$ where $k \in$ Integer.
   $\Rightarrow x^2 = (2k)^2$.
   $\Rightarrow x^2 = 4k^2 = 2(2k^2) \in$ Integer.
   $\Rightarrow x^2$ is even.
   x^2 is not odd.

b. The sum of two even integers is an even integer. Solution: If two even integers are added, then the result is an even integer. Proof (direct): $\forall x \forall y[x \text{ even} \wedge y \text{ even} \Rightarrow x + y \text{ even}]$
   x, y are even $\Rightarrow x = 2k, k \in$ Integers.
   $y = 2n, n \in$ Integers.
   $\Rightarrow x + y = 2k + 2n$.
   $\Rightarrow x + y = 2(k + n) \in I$.
   $\therefore x + y$ is even.

c. The sum of an even integer and an odd integer is an odd integer. Solution: If an even and odd number are added together, then the result is odd. $\forall x \forall y[x \text{ even} \wedge y \text{ odd} \Rightarrow x + y \text{ odd}]$.
   $x + y$ is odd $\Rightarrow x = 2k,\ k \in$ Integers.
   $y = 2n + 1, n \in I$.
   $\Rightarrow x + y = 2k + 2n + 1$.
   $\Rightarrow x + y = 2(k + n) + 1$.
   $\Rightarrow 2(k + n) + 1 \in$ Integer.
   $\therefore x + y$ is odd.

d. There are two odd integers whose sum is odd: Solution: $\exists x \exists y[x \text{ odd} \wedge y \text{ odd} \wedge x+y \text{ odd}]$. Show it is a false statement. Show $\neg\exists x \exists y[x \text{ odd} \wedge y \text{ even} \wedge x+y \text{ odd}]$ is true.
$\forall x \forall y \neg[(x \text{ odd} \wedge y \text{ odd}) \wedge x+y \text{ odd}]$.
$\forall x \forall y \neg[(x \text{ odd} \wedge y \text{ odd}) \vee \neg[x+y \text{ odd}]$.
$\forall x \forall y[(x \text{ odd} \wedge y \text{ odd}) \Rightarrow \neg[x+y \text{ odd}]$.
$\forall x \forall y[x \text{ odd} \wedge y \text{ odd} \Rightarrow x+y \text{ even}]$.
$x \text{ odd} \Rightarrow 2k+1, k \in I$.
$y \text{ odd} \Rightarrow 2n+1, n \in I$.
$x+y = 2k+2n+2 = 2(k+n+1), k+n+1 \in I$.
$\therefore x+y$ is even.

e. The square of any integer is negative. Solution: $\forall x[x^2 < 0]$ is false. If $x = 1, x^2 = 1 > 0$; $x = 1$ is a counter example.

g. There does not exist an integer x such that x^2+1 is negative. Solution: $\neg\exists x[x^2+1 < 0]$ true.
$\forall x \neg[x^2+1 < 0]$.
$\forall x[x^2+1 \geq 0]$.
$x^2 = x \times x \geq 0$.
$\Rightarrow x^2+1 \geq 0$.

i. If $1 = 3$, then the square of any integer is negative. Solution: Vacuous proof.

j. If $1 = 3$, then the square of any integer is positive. Solution: Vacuous proof.

k. The sum of any two primes is a prime number. Solution: 7, 11.

l. There exists two primes whose sum is prime: Solution: 2,3.

m. If the square of any integer is negative, then $1 = 1$. Solution: Vacuous proof.

1.2 Sets

A *set* is a collection of objects or elements. Capital letters denote sets and lower case letters denote elements of sets. To describe a set:

1. List elements $\{1, 2, 3\}$.
2. Set builder notation $\{x|x \text{ is a natural number}\}$.
$\{\frac{p}{q}|p \text{ and } q \text{ are integers and } q \neq 0\}$ = rational numbers.

The *null set* or the *empty set* is the set which contains no elements. This is denoted by $\emptyset$. The null set $\emptyset \neq \{\emptyset\}$. Sets can be:

1. Finite — has a last element.
2. Infinite

Sets A and B are equal ($A = B$) if they contain exactly the same elements $\{1, 2, 3\} = \{3, 2, 1\}$. $A = B$ iff every element in A is also in B and every element in B is also in A. $A = B$ iff $\forall x[(x \in A \Rightarrow x \in B) \wedge (x \in B \Rightarrow x \in A)]$.

A is a subset of B if every element of A is also an element of B. This is denoted by $A \subset B$. $A \subset B \Leftrightarrow \forall x[x \in A \Rightarrow x \in B]$. If $A \subset B$ then $B \supset A$.

Let U be a universal set. Then, $A \subset U$ for all sets A. Proof: $x \in A \Rightarrow x \in U$. $A \subset U$ by definition.

$(A = B)$ iff $(A \subset B \wedge B \subset A)$. Proof: Only if part (left to right) definition of subsets.

Corrolary: (falls directly from something proved) $A \subset A$. Proof: Since every set is equal to itself, then every set must be a subset of itself.

If $A \subset B$ and $B \subset C$, then $A \subset C$. Proof:
$A \subset B \Leftrightarrow x \in A \Rightarrow x \in B$.
$B \subset C \Leftrightarrow x \in B \Rightarrow x \in C$.
$A \subset C \Leftrightarrow x \in A \Rightarrow x \in C$.

Prove $\emptyset \subset A, \forall A$. Proof: $\emptyset \subset A \Leftrightarrow x \in \emptyset \Rightarrow x \in A$. Vacuous proof. $x \in \emptyset$ has no elements and therefore always false making the implication always true.

Let $\emptyset$ and $\emptyset'$ both be null sets. Then, $\emptyset = \emptyset'$. Proof: if $\emptyset$ is null, then $\emptyset \subset \emptyset'$. If $\emptyset'$ is null then $\emptyset' \subset \emptyset$. $\therefore \emptyset = \emptyset'$.

A *singleton* set is a set with exactly one element. For example, $S = \{a\}$. Result: every singleton set has exactly two subsets, the $\emptyset$ set and the subset itself. Result: $\emptyset$ has one subset, $\emptyset$.

Example: $S = \{a, b\}$. The subsets are $\emptyset, S, \{a\}, \{b\}$. (2^2).

Example: $S = \{a, b, c\}$ has 8 choices (2^3).

Example: $S = \{x_1, x_2, ..., x_n\}$ has 2^n.

A set with n elements has 2^n subsets.

Homework: page 79, 1-4 all, section 2.2 omit; section 2.3 page 84 1, 3, 4, 5.

Quiz # 3 — Friday October 9. 1 proof from Section 1.5. 2-3 problems from Sections 2.1 and 2.3.

Exam # 2 — Friday October 16. Section 1.5, 2.1, 2.3, 2.4.

1.2.1 Exam 2

1. Prove each of the following assertions using the method indicated.

   (a) The cube of an even integer is even. Direct proof. Solution: If x is even, then x^3 is even. Assume x is even,
   $\Rightarrow x = 2k$ where k is an integer
   $\Rightarrow x^3 = (2k)^3$
   $\Rightarrow x^3 = 8k^3$
   $\Rightarrow x^3 = 2(4k^3)$ where $4k^3 \in$ Integer
   $\therefore x^3$ is even.

   (b) If x is an odd integer, then x^2 is odd. Proof by contradiction. Solution: $\neg(x \text{ odd} \Rightarrow x^2 \text{ odd})$
   $\Leftrightarrow \neg(\neg x \text{ odd} \vee x^2 \text{ odd})$
   $\Leftrightarrow x \text{ odd} \wedge \neg x^2 \text{ odd}$
   $\Leftrightarrow x \text{ odd} \wedge x^2 \text{ even}$
   Let $x = 2k + 1$ where $k \in$ Integer
   Then, $x^2 = (2k + 1)^2 = 4k^2 + 4k + 1 = 2(2k^2 + 2k) + 1$
   where $2k^2 + 2k \in$ Integer

$\therefore x^2$ is odd which contradicts x^2 even.
$\therefore x^2$ is even.

(c) There is a prime number which is not odd. Constructive existence. Solution: Find a prime x such that $x = 2k$. 2 is an even prime number.

(d) If x^2 is an odd integer, then x is an odd integer. Indirect proof. Solution: if x is not odd, then x^2 is not odd. Assume x is not odd $\Rightarrow x$ is even
$\Rightarrow x = 2k$ where $k \in$ Integer
$\Rightarrow x^2 = (2k)^2$
$\Rightarrow x^2 = 4k^2$
$\Rightarrow x^2 = 2(2k^2)$ where $2k^2 \in$ Integer
$\therefore x^2$ is even.
$\therefore x^2$ is not odd.

2. Give all subsets of $\{\emptyset, \{1\}, 2\}$. Solution: $2^3 = 8$. $\emptyset$, $\{\emptyset\}$, $\{\{1\}\}$, $\{2\}$, $\{\emptyset, \{1\}\}$, $\{\emptyset, 2\}$, $\{\{1\}, 2\}$, and $\{\emptyset, \{1\}, 2\}$.

3. Draw a Venn diagram for $(A - B) \cup C$. See Figure 1.1.

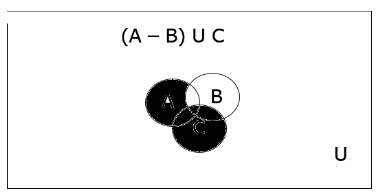

Figure 1.1: Venn diagram for problem 3a on Exam 2.

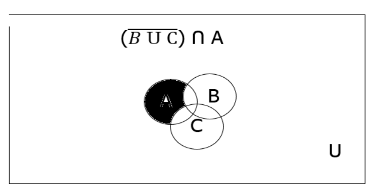

Figure 1.2: Venn diagram for problem 3b on Exam 2.

(a) Draw a Venn diagram for $\overline{(B \cup C)} \cap A$. See Figure 1.2.

4. Let $U = \{5, 6, 7, ..., 15\}$, $A = \{5, 9, 10, 11, 14\}$, $B = \{5, 7, 8, 9, 11, 15\}$, and $C = \{6, 7, 9, 10, 14, 15\}$. Give each of the following sets.

(a) $\overline{A} \cap B$. Solution: $\overline{A} = \{6, 7, 8, 12, 13, 15\}$. $\overline{A} \cap B = \{7, 8, 15\}$.

(b) $C - (A \cup B)$. Solution: $A \cup B = \{5, 7, 8, 9, 10, 11, 14, 15\}$. $C - (A \cup B) = \{6\}$.

(c) $\overline{(A \cap C)}$. Solution: $A \cap C = \{9, 10, 14\}$. $\overline{(A \cap C)} = \{5, 6, 7, 8, 11, 12, 13, 15\}$.

5. Prove the following identities.

(a) $A - \emptyset = A$. Solution: Let $x \in A - \emptyset \Leftrightarrow x \in A \wedge x \in \emptyset \Leftrightarrow x \in A \wedge 1 \Leftrightarrow x \in A$. $\therefore A - \emptyset = A$.

(b) $A \cup (\overline{A} \cap B) = A \cup B$. Solution: Let $x \in A \cup (\overline{A} \cap B)$. Then, $x \in A \vee x \in (\overline{A} \cap B) \Leftrightarrow x \in A \vee (x \notin A \wedge x \in B) \Leftrightarrow (x \in A \vee x \notin A) \wedge (x \in A \vee x \in B) \Leftrightarrow 1 \wedge (x \in A \vee x \in B) \Leftrightarrow x \subset A \vee x \in B \Leftrightarrow x \in A \cup B$
$\therefore A \cup (\overline{A} \cap B) = A \cup B$.

1.2.2 Quiz 3

1. Probe the following assertion by using a direct proof: The product of an even integer and an odd integer is even. Solution:
   x is even $\wedge y$ is odd $\Rightarrow x \cdot y$ even
   x even $\wedge$ y odd $\Rightarrow$
   $x = 2k$ where $k \in I$
   $y = 2n + 1$ where $n \in I$
   $\Rrightarrow x \cdot y = 2k(2n + 1)$
   $\Rightarrow x \cdot y = 4kn + 2k$
   $\Rightarrow x \cdot y = 2(2kn + k)$
   $\Rightarrow (2k + k) \in I$
   $\therefore x \cdot y$ even.

2. List all subsets of $\{\{2\}, 5\}$. Solution: $\emptyset$, $\{\{2\}, 5\}$, $\{\{2\}\}$, $\{5\}$.

3. Let $S = \{4, 5, 9, 12, 14, 20\}$. How many subsets does S have? Solution: $2^6 = 64$ subsets.

4. Disprove the following statements by finding a counterexample for each.

   (a) $(A \in B \wedge B \notin C) \Rightarrow A \notin C$. Solution: $A \in B \wedge B \notin C \wedge A \in C$.

   (b) $(A \subset B \wedge A \subset C) \Rightarrow B \subset C$. Solution: $A = \{1\}$, $B = \{1, 2, 3\}$, $C = \{1, 2, 4\}$.

1.2.3 Operations on Sets

The *union* of sets A and B is $A \cup B = \{x | x \in A \vee x \in B\}$. The *intersection* of sets A and B is $A \cap B = \{x | x \in A \wedge x \in B\}$. The difference of sets A and B is $A - B = \{x | x \in A \wedge x \notin B\}$.

Example: $A = \{1, 2, 3, 4, 5\}$. $B = \{2, 4, 6\}$. $A \cup B = \{1, 2, 3, 4, 5, 6\}$. $A \cap B = \{2, 4\}$. $A - B = \{1, 3, 5\}$.

Sets A and B are called *disjoint* if they have no elements in common. $A \cap B = \emptyset$. A collection, C, of sets in which any two elements are disjoint is called a collection of *pairwise disjoint sets.*

Example: $C = \{\{1, 2, 3\}, \{4\}, \{5, 6\}\}$.

The union and intersection are both commutative and associative operations. $A \cup B = B \cup A$ is commutative. $A \cap B = B \cap A$ is commutative. $A \cup (B \cup C) = (A \cup B) \cup C$ is associative and $A \cap (B \cap C) = (A \cap B) \cap C$ is associative. Proof:
Show that $A \cap B = B \cap A$.
$x \in A \cap B \Leftrightarrow x \in A \wedge x \in B$.
$\Leftrightarrow x \in B \wedge x \in A$.
$\Leftrightarrow x \in B \cap A$.

Recall:

1. $R \subset S \Leftrightarrow x \in R \Rightarrow x \in S$.

2. If $R \subset S$ and $S \subset R$, then $R = S$.

The union and intersection distribute over each other. $A \cup (B \cap C) = (A \cup B) \cap (A \cup C)$ and $A \cap (B \cup C) = (A \cap B) \cup (A \cap C)$. Proof:
$A \cup (B \cap C) = (A \cup B) \cap (A \cup C)$
$x \in A \cup (B \cap C) \Leftrightarrow x \in A \vee x \in (B \cap C)$
$\Leftrightarrow x \in A \vee [x \in B \wedge x \in C]$
$\Leftrightarrow (x \in A \vee x \in B) \wedge (x \in A \vee x \in C)$
$\Leftrightarrow x \in (A \vee B) \wedge x \in (A \cup C)$

$\Leftrightarrow x \in (A \cup B) \cap (A \cup C)$
$\therefore A \cup (B \cap C) = (A \cup B) \cap (A \cup C)$

Page 88, Theorem 2.43: Show that $A \cup \emptyset = A$. Proof:
$x \in (A \cup \emptyset) \Leftrightarrow x \in A \vee x \in \emptyset$.
$\Leftrightarrow x \in A \vee \emptyset$.
$\Leftrightarrow x \in A$.
$\therefore A \cup \emptyset = A$.

Theorem: $A - B \subset A$. Proof:
$x \in A - B \Leftrightarrow x \in A \wedge x \notin B$.
$\Rightarrow x \in A$.
$\therefore A - B \subset A$.

Theorem: $A \subset A \cup B$. Proof:
$x \in A \Rightarrow x \in A \vee x \in B$.
$\Leftrightarrow x \in A \cup B$.
$\therefore A \subset A \cup B$.

1.2.4 Homework and Answers

Section 2.1, page 79 1-4 in the textbook.

1. Specify the following sets explicitly.

a. The set of non-negative integers less than 5. Solution: $\{0, 1, 2, 3, 4\}$.

b. The set of letters in your first name. Solution: $\{r, o, g, e, r\}$.

c. The set whose only element is the first president of the United States. Solution: $\{washington\}$.

d. The set of prime numbers between 10 and 20. Solution: $\{11, 13, 17, 19\}$.

e. The set of positive multiples of 12 which are less than 65. Solution: $\{12, 24, 48, 60\}$.

2. For each of the following, choose an appropriate universe of discourse and a predicate to define the set. Do not use ellipses.

a. The set of integers between 0 and 100. Solution: $\{x|x > 0 \wedge x < 100\}$.

b. The set of odd integers. Solution: $\{x|\exists y[x = 2y + 1]\}$.

c. The set of integer multiples of 10. Solution: $\{x|\exists y[x = 10y]\}$.

d. The set of human fathers. Solution: $U =$ all humans. $\{x|x \text{ is a father }\}$.

e. The set of tautologies. Solution: $U =$ tautalogies.

3. List the members of the following sets.

a. $\{x|x \in I \wedge 3 < x < 12\}$. Solution: $\{4, 5, 6, 7, 8, 9, 10, 11\}$.

c. $\{x|x = 2 \vee x = 5\}$. Solution: $\{2, 5\}$.

4. Determine which of the following sets are equal. The universe of discourse is I. $A = \{x|x \text{ is even and } x^2 \text{ is odd}\}$. $B = \{x|\exists y[y \in I \wedge x = 2y]\}$. $C = \{1, 2, 3\}$. $D = \{0, 2, -2, 3, 4, -4, ...\}$. $E = \{2x|x \in I\}$. $F = \{3, 3, 2, 1, 2\}$. $G = \{x|x^3 - 6x^2 - 7x - 6 = 0\}$. Solution: $A = \emptyset$. $B = \{-4, -2, 0, 2, 4\}$. $C = \{1, 2, 3\}$. $D = \{0, 2, -2, 3, -3, 4, -4, ...\}$. $E =$ evens. $F = \{3, 2, 1\}$. $G = \emptyset$. Result $\frac{p}{a}$ where p is a factor of a_0 and a is a factor of a_n. $B = E$, $C = F$, and $A = G$.

1.2.5 Homework and Answers

Page 84: Section 2.3, problems 1, 3, 4, 5 in the textbook.

1. List all alphabets of the following sets.

a. $\{1, 2, 3\}$. Solution: $2^3 = 8$. $\{1\}$, $\{2\}$, $\{3\}$, $\{1, 2\}$, $\{1, 3\}$, $\{2, 3\}$, $\{1, 2, 3\}$, $\emptyset$.

b. $\{1, \{2, 3\}\}$. Solution: 2^2. $\emptyset$, $\{1\}$, $\{\{2, 3\}\}$, $\{1, \{2, 3\}\}$.

c. $\{\{1, \{2, 3\}\}\}$. Solution: $\emptyset$, $\{\{1, \{2, 3\}\}$.

d. $\emptyset$, Solution: $\{\emptyset\}$.

e. $\{\emptyset, \{\emptyset\}\}$, Solution: $\emptyset$, $\{\emptyset\}$, $\{\{\emptyset\}\}$.

3. Let A, B and C bet sets. If $A \in B$ and $B \in C$, is it possible that $A \in C$? Is it always true that $A \in C$? Give examples to support your assertions. Solution: Yes $A = \{1\}$. No $B = \{2, \{5, 6\}, \{1\}\}$. Not always true $C = \{\{1\}, \{2, \{5, 6\}\}\}$. $A \in B$, $B \in C$. $\therefore A \in C$.

5. Briefly describe the differnce between the sets $\{2\}$ and $\{\{2\}\}$. List the elements and all the subsets of each set. Solution: $\{2\}$ contains the element 2. $\{\{2\}\}$ contains the set $\{2\}$. The type of element is different. The set $\{2\}$ has the subsets $\emptyset, \{2\}$. The set $\{\{2\}\}$ has the subset $\{2\}$.

1.2.6 Homework and Answers

Page 88 Theorem 2.4.3 prove parts (m), (n), and (p).

m. Prove $A \cap (B - A) = \emptyset$. Solution:
$x \in A \cap (B - A) \Leftrightarrow$
$x \in A \wedge x \in (B - A) \Leftrightarrow$
$x \in A \wedge (x \in B \wedge x \notin A) \Leftrightarrow$
$(x \in A \wedge x \notin A) \wedge x \in B \Leftrightarrow$
$0 \wedge x \in B \Leftrightarrow$
$0 \Leftrightarrow$
$x \in \emptyset$
$\therefore A \cap (B - A) = \emptyset$.

n. Prove $A \cup (B - A) = A \cup B$. Solution:
$x \in A \cup (B - A) \Leftrightarrow$
$x \in A \vee x \in (B - A) \Leftrightarrow$
$x \in A \vee (x \in B \wedge x \notin A) \Leftrightarrow$
$(x \in A \vee x \in B) \wedge (x \in A \vee x \notin A) \Leftrightarrow$
$(x \in A \vee x \in B) \wedge 1 \Leftrightarrow$
$x \in A \vee x \in B$
$x \in (A \cup B)$.

p. Prove $A - (B \cap C) = (A - B) \cup (A - C)$. Solution:
$x \in A - (B \cap C) \Leftrightarrow$
$x \in A \wedge x \notin (B \cap C) \Leftrightarrow$
$x \in A \wedge \neg x \in (B \cap C) \Leftrightarrow$
$x \in A \wedge \neg(x \in B \wedge x \in C) \Leftrightarrow$
$x \in A \wedge (\neg x \in B \vee \neg x \in C) \Leftrightarrow$
$(x \in A \wedge \neg x \in B) \vee (x \in A \wedge \neg x \in C) \Leftrightarrow$
$(x \in A \wedge x \notin B) \vee (x \in A \wedge x \notin C) \Leftrightarrow$

$(x \in (A - B)) \vee (x \in (A - C)) \Leftrightarrow$
$x \in (A - B) \cup (A - C) \Leftrightarrow$
$\therefore A - (B \cap C) = (A - B) \cup (A - C)$.

1.2.7 Complement of Sets

Let $A \subset U$. Then, the *complement* of A is denoted by $\bar{A}$ and is given by $\bar{A} = U - A = \{x | x \notin A\}$.

Example: Let $U = \{1, 2, 3, 4, 5\}$ and $A = \{2, 5\}$. Then, $\bar{A} = \{1, 3, 4\}$.

Let $A \subset U$. Then the following statements are true:

1. $A \cup \bar{A} = U$.
2. $A \cap \bar{A} = \emptyset$.

Proof: $A \cup \overline{A} = U$.
$x \in A \cup \overline{A} \Leftrightarrow$
$x \in A \vee x \in \overline{A} \Leftrightarrow$
$x \in A \vee x \notin A \Leftrightarrow$
$1 \Leftrightarrow$
$x \in U$.
$\therefore A \cup \overline{A} = U$.

Proof: $A \cap \overline{A} = \emptyset$. Let $A \subset U \wedge B \subset U$. Then, $B = \overline{A}$ iff $A \cup B = U \wedge A \cap B = \emptyset$. Proof (only part):
If $B = \overline{A}$, then $A \cup B = A \cup \overline{A} = U \wedge A \cap B = A \cap \overline{A} = \emptyset$. If $A \cup B = U \wedge A \cap B = \emptyset$, then $B = \overline{A}$.
$B = U \cap B$
$= (A \cup \overline{A}) \cap B$
$= (A \cap B) \cup (\overline{A} \cap B)$
$= \emptyset \cup (\overline{A} \cap B)$
$= (\overline{A} \cap A) \cup (\overline{A} \cap B)$
$= \overline{A} \cap (A \cup B)$
$= \overline{A} \cap U$
$= \overline{A}$.

Let $A \subset U$. Then, $\overline{\overline{A}} = A$.

1.2.8 Venn Diagrams

This section covers Venn diagrams and De'Morgan's laws. Let $A \subset U \wedge B \subset U$. Then, the following are *De'Morgan's Laws:*

1. $\overline{A \cup B} = \overline{A} \cap \overline{B}$.
2. $\overline{A \cap B} = \overline{A} \cup \overline{B}$.

Venn diagrams are used to represent set operations. See Figures 1.3 thru 1.8.

Do problems 1a, b and 10 on page 92.

1.2.9 Homework and Answers

Page 92 of the textbook.

1. Construct Venn diagrams for each of the following.

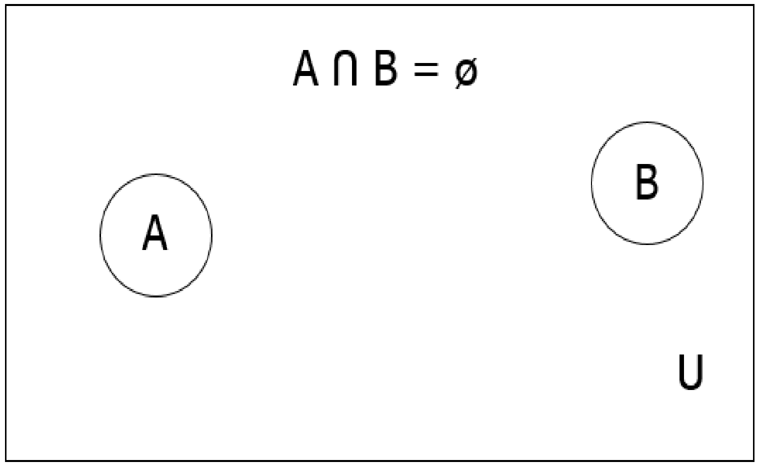

Figure 1.3: Venn diagram of the intersection of two sets being the null value.

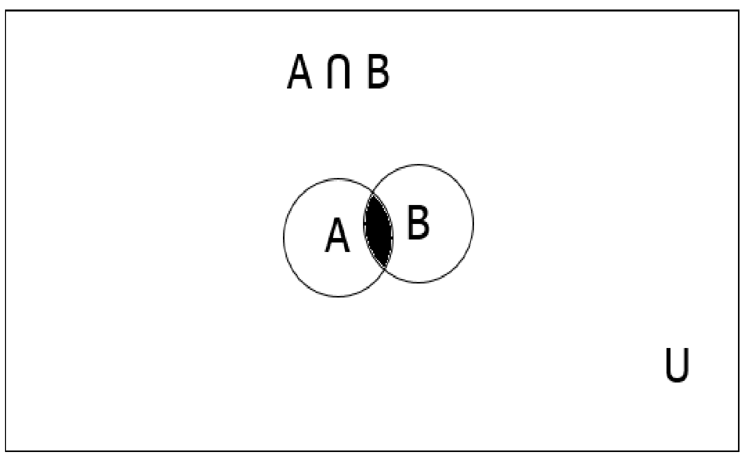

Figure 1.4: Venn diagram of the intersection of two sets.

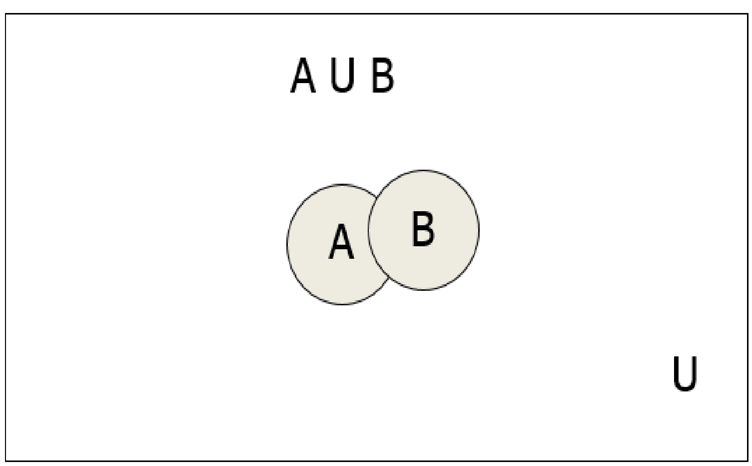

Figure 1.5: Venn diagram of the union of two sets.

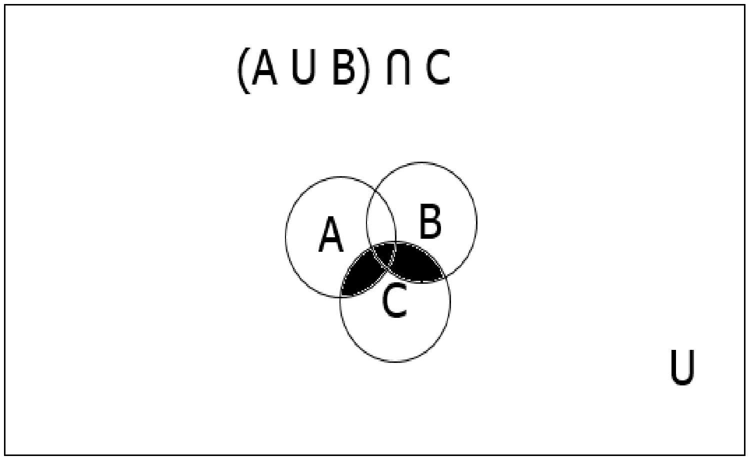

Figure 1.6: Venn diagram of a complicated intersection.

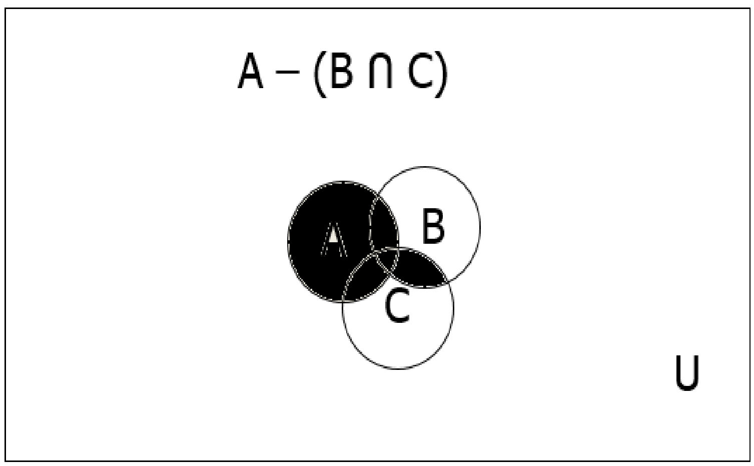

Figure 1.7: Venn diagram of a complicated negation.

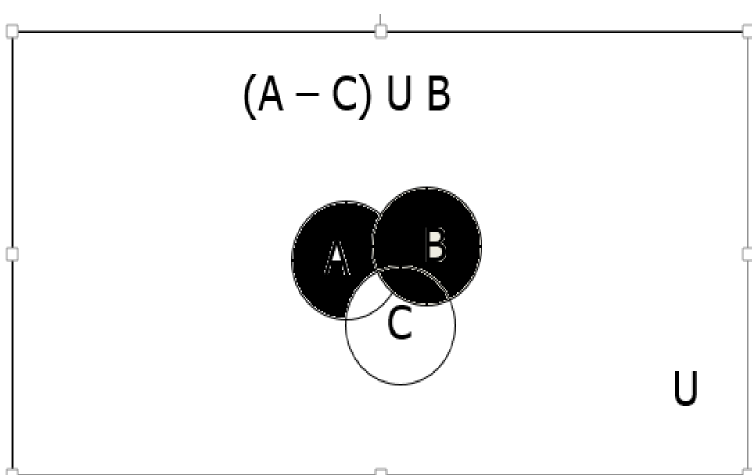

Figure 1.8: Venn diagram of negation and union.

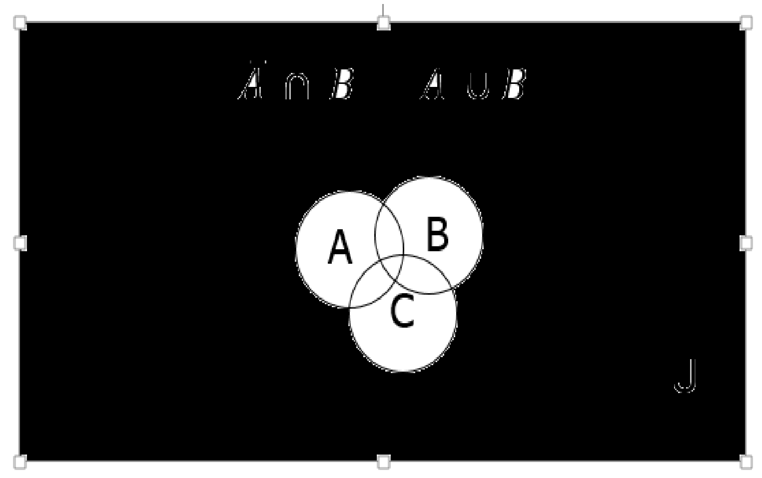

Figure 1.9: Venn diagram of Problem 1a $\overline{A} \cap \overline{B} = \overline{A \cup B}$.

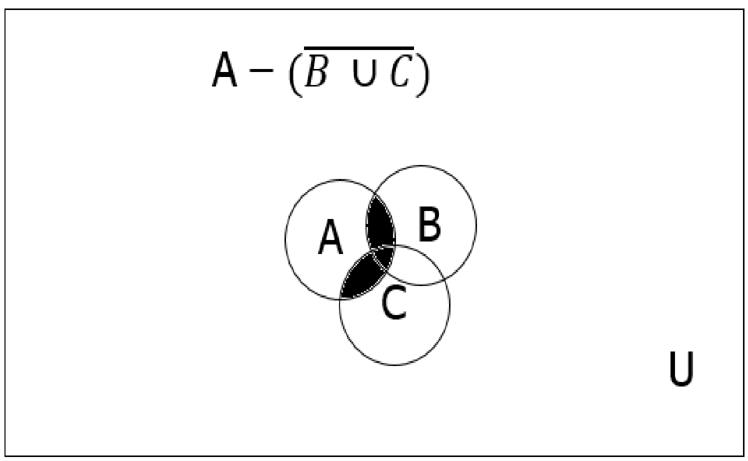

Figure 1.10: Venn diagram of Problem 1a $A - (\overline{B \cup C})$.

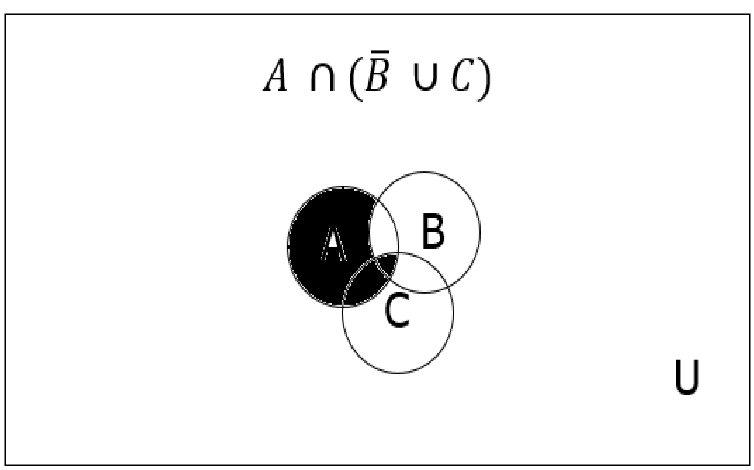

Figure 1.11: Venn diagram of Problem 1a $A \cap (\overline{B} \cup C)$.

a. $A \cup B$. Solution: See Figure 1.5. $\overline{A} \cap \overline{B} = \overline{A \cup B}$. See Figure 1.9. $A - (\overline{B \cup C})$. See Figure 1.10. $A \cap (\overline{B} \cup C)$. See Figure 1.11.

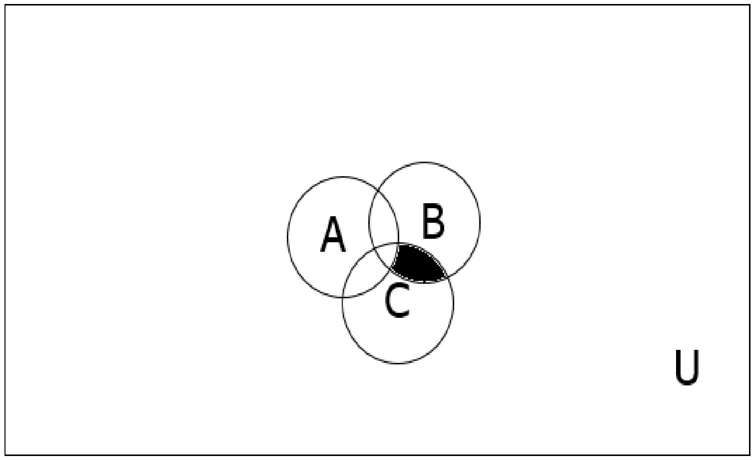

Figure 1.12: Venn diagram of Problem 1b (i).

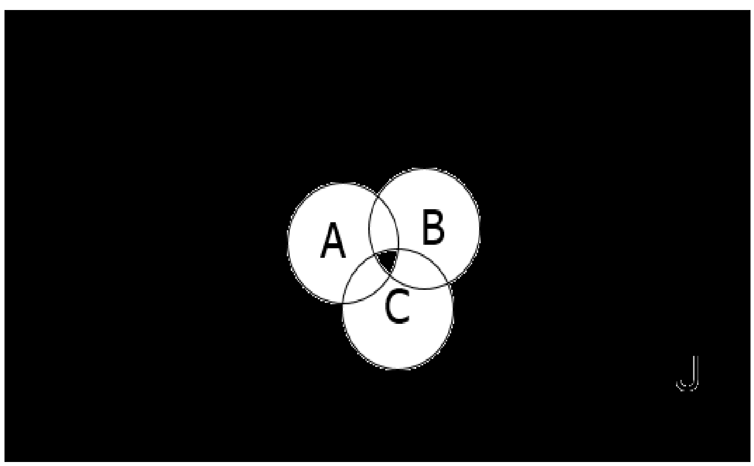

Figure 1.13: Venn diagram of Problem 1b (ii).

b. Give a formula which denotes the shaded portion of each of the following Venn diagrams. Solution: See Figure 1.12. (i) $(B \cap C) - A$. See Figure 1.13. (ii) $(\overline{A \cup B \cup C}) \cup (A \cap B \cap C)$. See Figure 1.14. (iii) $\emptyset$.

10. Prove the following identities.

a. $A \cup (A \cap B) = A$. Solution:
$x \in A \cup (B \cap A)$
$x \in (A \vee (B \wedge A))$
$x \in (A \vee B) \wedge x \in (A \vee A)$
$x \in (A \vee B) \wedge x \in A$
$x \in (A \wedge A) \vee x \in (A \wedge B)$
$x \in A \vee x \in (A \wedge B)$.

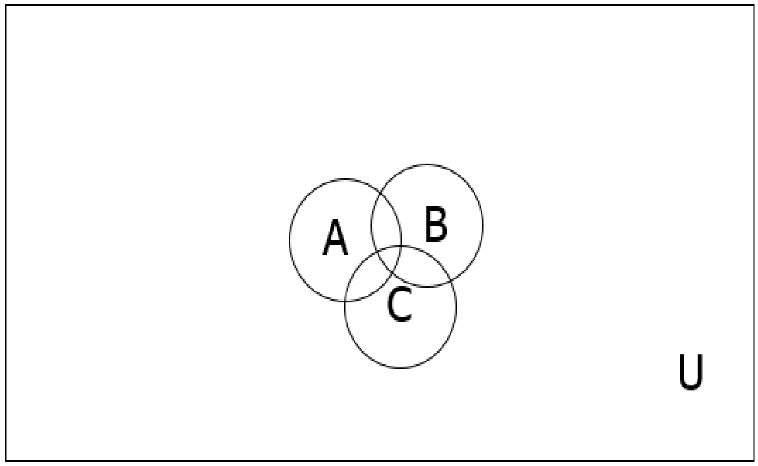

Figure 1.14: Venn diagram of Problem 1b (iii).

b. $A \cap (A \cup B) = A$. Solution:
$x \in A \cap (A \cup B)$
$x \in A \wedge x \in (A \vee B)$
$(x \in A \wedge x \in A) \vee (x \in A \wedge x \in B)$
$x \in A \vee x \in (A \wedge B)$
$x \in A$
$\therefore A$.

c. $A - B = A \cap \overline{B}$. Solution:
$x \in A - B$
$x \in A \wedge x \notin B$
$x \in A \cap \overline{B}$
$A \cap \overline{B}$.

d. $A \cup (\overline{A} \cap B) = A \cup B$. Solution:
$x \in A \cup (\overline{A} \cap B)$
$x \in A \vee (x \notin A \wedge x \in B)$
$(x \in A \vee x \notin A) \wedge (x \in A \vee x \in B)$
$1 \wedge x \in (A \vee B)$
$x \in (A \cup B)$
$(A \cup B)$.

e. $A \cap (\overline{A} \cup B) = A \cap B$. Solution:
$x \in A \cap (\overline{A} \cup B)$
$x \in A \cap x \in (\overline{A} \cup B)$
$x \in A \cap (x \notin A \cup x \in B)$
$x \in A \wedge (x \notin A \vee x \in B)$
$(x \in A \wedge x \notin A) \vee (x \in A \wedge x \in B)$
$0 \vee (x \in A \wedge x \in B)$
$x \in (A \wedge B)$
$x \in (A \cap B)$
$A \cap B$.

1.2.10 Generalized Unions and Intersections

Test on Section 1.5. Direct proof, indirect proof, vacuous proof, trivial proof, contradition proof, constructive proof. Section 2.1, 2.3 and 2.4. Set operations, subsets and Venn diagrams. Prove page 88 but not f and g.

If C is a non-empty collection of subsets of U, then

1. The union of the elements of C is $\cup_{s\in C} S = \{x | \exists s[s \in C \wedge x \in S\}$.

   Example: $C = \{\{1,2,3\},\{3,4\},\{2,5,8\}\}$. $\cup_{s\in C} S = \{1,2,3,4,5,8\}$.

2. The intersection of the elements of C is $\cap_{s\in C} S = \{x | \forall s \ \ s \in C \Rightarrow x \in S\}$.
   Also, $\cap_{s\in C} S = \emptyset$.

The *power set* of a set A is denoted by $P(A)$ and is the set of all subsets of A.

Example: $A = \{a, b\}$. $P(A) = \{\emptyset, \{a, b\}, \{a\}, \{b\}\}$.

Do problems 11, 14, and 15 on page 94 in the textbook.

1.2.11 Induction

Inductively defined sets are all infinite. An *inductive definition* has 3 components:

1. *The basis clause* — it establishes that certain elements are in the set.

2. *The inductive clause* — this describes how elements of the set can be combined to form new elements of the set.

3. *The extremal clause* — this asserts that the only elements in the set are those which can be generated by applying clauses (1) and (2) a finite number of times.

Example: Define the set of even, non-negative integers $E = \{0, 2, 4, 6, ...\}$.

1. Basis — $0 \in E$.

2. Inductive — If $n \in E$, then $n + 2 \in E$.

3. Extremal — All elements in E can be generated by a finite number of applications of caluses (1) and (2).

Prove that $8 \in E$. Solution:
$0 \in E$. Basis
$0 \in E \Rightarrow 0 + 2 \in E$. Inductive
$2 \in E \Rightarrow 2 + 2 \in E$. Inductive
$4 \in E \Rightarrow 4 + 2 \in E$. Inductive
$6 \in E \Rightarrow 6 + 2 \in E$. Inductive

An *alphabet* denoted by Σ is a finite non-empty set of symbols or characters. A *word* or *a string* over Σ is a string of finite number of symbols from Σ.

Example: If $x = a_1a_2\cdots a_n$ is a string over sigma (Σ), the length of x is n.

The *null string* or *empty string* is denoted by Λ and is the string of length 0. If x and y are strings over Σ and $x = a_1a_2\cdots a_n$ and $y = b_1b_2\cdots b_m$, then x *concatenated* with y is denoted by xy is the string $xy = a_1a_2\cdots a_nb_1b_2\cdots b_m$. Note that concatenation is not commutative. If Σ is an alphabet, then Σ^+ denotes a set of all non-empty strings over sigma (Σ).

1. Basis — if $a \in \Sigma$, then $a \in \Sigma^+$.
2. Inductive — if $x \in \Sigma^+$, and $a \in \Sigma$, then $ax \in \Sigma^+$.
3. Extremal — Σ^+ contains only those strings which can be generated by a finite number of applications of (1) and (2).

Example: $\Sigma = \{a, b\}$. Prove $babba \in \Sigma^+$. Go right-to-left.
$a \in \Sigma^+$. Basis
$ba \in \Sigma^+$. Inductive
$bba \in \Sigma^+$. Inductive
$abba \in \Sigma^+$. Inductive
$babba \in \Sigma^+$. Inductive

The *transitive closure* Σ^* of Σ is the set of all finite length strings over Σ. $\Sigma^* = \Sigma^+ \cup \{\Lambda\}$. The inductive definition of Σ^* is as follow:

1. Basis — $\Lambda \in \Sigma^*$.
2. Inductive — If $x \in \Sigma^*$ and $a \in \Sigma$, then $ax \in \Sigma^*$.
3. Extremal — The same.

For any string x over Σ, $x\Lambda = \Lambda x = x$.

Example: $\Sigma = \{a, b\}$. $\Sigma^* = \{\Lambda, a\Lambda, b\Lambda, ...\}$.

1.2.12 Inductive Definition of Sets

This section covers the bottom of page 97 of the textbook and page 98, part A.

Let S equal to well formed arithmetic expressions. $S = \{0, 1, 2, ..., 9, 10, 11, 12, 13, ..., (+0), (2 + 9), \left(\frac{31}{42}\right), \left((2 + 0 \times \left(\frac{31}{42}\right)\right), ...\}$. Part B: $V = \{P, Q, R, ...\}$.. Basis: $\{0, 1, P, Q, R, (P \vee Q), (\neg(P \vee Q))$.

Inductive proofs: These are proofs of assertions of the form $\forall x P(x)$. The universe is inductively defined. The proofs have 2 parts:

1. Basis — show that $P(x)$ is true for all elements in the basis part of the definition.
2. Induction — show that every element obtained using the indutive clause of the difinition satisfies $P(x)$ of all elements used in its construction also satisfies $P(x)$.

Example: Let $U =$ natural numbers $= \{0, 1, 2, ...\}$. The natural numbers N are defined as follow:

1. $0 \in N$.
2. If $n \in N$, then $n + 1 \in N$.
3. Same.

To use this definition to prove $\forall x P(x)$, show that

1. $P(0)$ is true
2. Show $\forall n[P(n) \Rightarrow P(n + 1)]$.

This is called the *first principle of mathematical induction.*

Example: $\forall n \in N$. $\sum_{i=0}^{n} i = \frac{n(n+1)}{2}$. Proof:

1. If $n = 0$, $\sum_{i=0}^{0} = \frac{0(1)}{2} = 0 = 0$.
2. Assume $P(n)$ is true. Show that $P(n+1)$ is also true.

$$\sum_{i=0}^{n+1} i = (n+1) + \sum_{i=0}^{n} i =$$

$$\frac{2(n+1)}{2} + \frac{n(n+1)}{2} =$$

$$\frac{2(n+1) + n(n+1)}{2} =$$

$$\frac{(n+1)(n+2)}{2}$$

$\therefore \forall n P(n)$.

For the first principle of mathematical induction over natural numbers:

(a) Show that $P(0)$ is true.

(b) Assume $P(n)$ is true, then show $P(n+1)$ is true.

Applied to binary trees, this gives the following result. If a binary tree has n nodes, then there are $n+1$ nil pointers. Proof:

(a) If $n = 1$, then there are 2 nil pointers.

(b) Assume if there n nodes, then there are $n+1$ nil pointers. Show if there are $n+1$ nodes then there are $n+2$ nil pointers. Add 1 node to a tree with n nodes. The original tree had $n+1$ nil pointers. By adding 1 node, one nil pointer is lost, but 2 nil pointers are gained. So, the total gain is 1 nil pointer. $\therefore$ There are now $n+2$ nil pointers.

The *second principle of induction:* Assume $P(k)$ is true for all $k < n$. Show that $P(n)$ is also true.

```
procedure inorder(p: pointer);
begin
if p <> nil then
begin
inorder(p↑ .left);
process(p);
inorder(p↑ .right);
end;
end;
```

Prove that the procedure INORDER correctly visits the nodes in a tree of size n. Proof: Assume that INORDER works correctly on all trees with fewer than n nodes. Each node has at most $n-1$ nodes.

1.2.13 Set Operations on Σ^*

Set operations on Σ^*, where Σ^* is equal to the set of all finite length strings over Σ (chosen characters). Note that $\Lambda \in \Sigma^*$. Let $x \in \Sigma^*$ and $n \in N$, then

(a) Basis — $x^0 = \Lambda$.

(b) Induction — $x^{n+1} = x^n x$.

Example: $\Sigma = \{a, b, c\}$. Choose $x = abc \in \Sigma^*$.
$x^0 = (abc)^0 = \Lambda$
$x^1 = x^0 \cdot x = \Lambda \cdot x = abc$
$x^2 = x^1 \cdot x = abc \cdot abc = abcabc$.

Example: $\{(a, b)^n | n \geq 0\} = \{\Lambda, ab, abab, ababab, ...\}$.

Example: $\{(a^n b^n | n \geq 0\} = \{\Lambda, ab, aabb, aaabbb, ..., \}$.

Let Σ be a finite alphabet. Then a language over Σ is any subset of Σ^*.

Example: $\Sigma = \{a, b, c\}$. Let $A = \{ab, acc, b, ca\}$. A is a *language* over Σ.

Σ is equal to the set of ASCII characters. Σ^* is equal to all finite strings of ASCII characters. Let A equal to the set of all legal Pascal commands or programs. If A and B are languages over Σ, then the *set product* of A with B is the language consisting of all strings formed by concatinating an element of A with an element of B.

Example: $\Sigma = \{a, b, c\}$. $A = \{a, bc\}$. $B = \{\Lambda, b, ac\}$. Then, $AB = \{a, ab, aac, bc, bcb, bcac\}$. Also, $AB \neq BA$.

Quiz on Monday: Induction and sets. Don't have to know Section 2.7.1 on 113. Know Section 2.7.3 on page 115. Have to know 1 induction proof like the one on page 107 #4 and 6. Given an induction definition — work with it — prove an element is in the set. Know Section 2.5 and 2.7

1.2.14 Homework and Answers

Page 106 - 107, 1, 3, 4, 6a, b, c in the textbook.

1. Give inductive definitions for the following sets.

a. The set of unsigned integers in decimal representation. The defined set should include 4, 167, 0012, etc. Solution: Unsigned integers equals to S. Basis: let $D = \{0, 1, 2, ..., 9\}$. If $d \in D$, then $d \in S$. Induction: If $x \in S$, and $d \in D$, then $xd \in S$. External: 271 is an unsigned integer. So, Step:

   (a) $2 \in S$.
   (b) $2 \in S$, $7 \in D \Rightarrow 27 \in S$.
   (c) $27 \in S$, $1 \in D \Rightarrow 271 \in S$.

b. The set of real numbers with terminating fractional parts in decimal representation. The defined set should include 6.1, 712., 01.2100, 0.190, etc. Solution: Real number with terminating fractional parts equal to S. Basis: let $D = \{0, 1, 2, ..., 9\}$. If $d \in D$, then $d\cdot \in S$ and $\cdot d \in S$. Induction: If $x \in S$ and $d \in D$, then $xd \in S$ and $dx \in S$. Extremal: consider 21.68. So,
Step:

   (a) $1. \in S$.
   (b) $1. \in S \wedge 2 \in D \Rightarrow 21. \in S$.
   (c) $21. \in S \wedge 6 \in D \Rightarrow 21.6 \in S$.
   (d) $21.6 \in S \wedge 8 \in D \Rightarrow 21.68 \in S$.

3. Give an inductive definition of $n!$ and use it to prove the identity

$$n! = \prod_{i=1}^{n} i.$$

Solution: $n! = n(n-1)(n-2)\cdots 3 \cdot 2 \cdot 1$. Basis: $1! = 1$. Induction: show $\prod_{i=1}^{n+1} i = (n+1)!$

$$\begin{aligned}
&\prod_{i=1}^{n+1} i = (n+1)\prod_{i=1}^{n} i = \\
&(n+1)n! = \\
&(n+1)!
\end{aligned}$$

4. Prove by induction that $(1+2+3+\cdots+n)^2 = 1^3+2^3+3^3+\cdots+n^3$ for all $n \in I+$. Solution: Proof basis case. $n=1$, $P(1) = 1^2 = 1^3 = 1$. Induction: Assume $P(n)$ is true. Show $P(n+1)$ is true.

$$\begin{aligned}
&P(n+1) = \\
&(1+2+\cdots+n+(n+1))^2 = \\
&(1^3+2^3+3^3+\cdots+(n+1)^3) = \\
&(1+2+\cdots+n+1)^2 = \\
&((1+2+\cdots+n)+(n+1))^2 = \\
&(1+2+3+\cdots+n)^2 + 2(1+2+\cdots+n)(n+1) + (n+1)^2 = \\
&1^3+2^3+\cdots+n^3 + \frac{2n(n+1)(n+1)}{2} + (n+1)^2 = \\
&1^3+2^3+\cdots+n^3 + n(n+1)^2 + (n+1)^2 = \\
&1^3+2^3+\cdots+n^3 + (n+1)^2(n+1) = \\
&1^3+2^3+\cdots+n^3 + (n+1)^3.
\end{aligned}$$

6. Prove each of the following relationships for all $n \in N$.

a. $\sum_{i=0}^{n} i^2 = \frac{n(n+1)(2n+1)}{6}$. Basis: $n=0$. $\sum_{i=0}^{0} i^2 = \frac{0(0+1)(0+1)}{6} = 0 = 0$. Induction: Assume $\sum_{i=0}^{n} i^2 = \frac{n(n+1)(2n+1)}{6}$. Show that $\sum_{i=0}^{n+1} i^2 = \frac{(n+1)(n+2)(2n+3)}{6}$.

$$\begin{aligned}
&\sum_{i=0}^{n+1} i^2 = (n+1)^2 + \sum_{i=0}^{n} i^2 = \\
&(n+1)^2 + \frac{n(n+1)(2n+1)}{6} = \\
&\frac{6(n+1)^2}{6} + \frac{n(n+1)(2n+1)}{6} = \\
&\frac{6(n+1)^2 + n(n+1)(2n+1)}{6} = \\
&\frac{(n+1)[6(n+1)+n(2n+1)]}{6} = \\
&\frac{(n+1)[6n+6+2n^2+n]}{6} = \\
&\frac{(n+1)[2n^2+7n+6]}{6} = \\
&\frac{(n+1)(n+2)(2n+3)}{6}.
\end{aligned}$$

b. $\sum_{i=0}^{n}(2i+1) = (n+1)^2 = P(n)$. Solution: For the basis case, show that $P(0) = 0$. $\sum_{i=0}^{0}(2i+1) = (0+1)^2$, $1 = 1$. For the induction case, show $P(n+1)$ is also true.

$$P(n+1) = \sum_{i=0}^{n+1}(2i+1) = (n+2)^2$$

$$\sum_{i=0}^{n+1}(2i+1) = (2(n+1)+1) + \sum_{i=0}^{n} 2i+1 =$$

$$(2n+3) + (n+1)^2$$

$$2n+3+n^2+2n+1 =$$

$$n^2+4n+4 =$$

$$(n+2)^2.$$

c. $\sum_{i=0}^{n} i(i!) = (n+1)! - 1$. Solution: Show $\sum_{i=0}^{n} i(i!) = (n+1)! - 1$. Basis: if $n = 0$, $\sum_{i=0}^{0} i(i!) = (0+1)! - 1 = 0(0!) - 1 = 0 = 0$. Induction: Assume that $\sum_{i=0}^{n} i(i!) = (n+1)! - 1$. Show $\sum_{i=0}^{n+1} i(i!) = (n+2)! - 1$.

$$\sum_{i=0}^{n+1} i(i!) =$$

$$(n+1)(n+1)! + \sum_{i=0}^{n} i(i!) =$$

$$(n+1)(n+1)! + (n+1)! - 1 =$$

$$(n+1)![(n+1)+1] - 1 =$$

$$(n+1)![(n+2)] - 1 =$$

$$(n+2)! - 1.$$

1.3 Binary Relations

An ordered $n-$tuple is a sequence of n objects denoted by $< a_1, a_2, ..., a_n >$ where a_i represents the i^{th} component of the n tuple. If $n = 2$, we have an *ordered pair.* If $n = 3$, we have an *ordered triple.* The *Cartesian product* of sets A_1, A_2, ... A_n is denoted by $A_1 \times A_2 \times A_3 \times \cdots \times A_n$ and is given by $\{< a_1, a_2, ..., a_n > | a_i \in A_i\}$.

Example: $A = \{2, 4\}$. $B = \{a, b, c\}$. $A \times B = \{< 2, a >, < 2, b >, < 2, c >, < 4, a >, < 4, b >, < 4, c >\}$. $B \times A = \{< a, 2 >, < b, 2 >, < c, 2 >, < a, 4 >, < b, 4 >, < c, 4 >\}$. $A \times B \neq B \times A$. Let $C = \{6\}$. $ABC = A \times B \times C = \{< 2, a, 6 >, < 2, b, 6 >, < 2, c, 6 >, < 4, a, 6 >, < 4, b, 6 >, < 4, c, 6 >\}$. $A^2 = A \times A = \{< 2, 2 >, < 2, 4 >, < 4, 2 >, < 4, 4 >\}$. $A^n = A \times A \times A \times \cdots \times A$.

$\Re$ equals to the real numbers. $\Re^2 = R \times R = \{< x, y > | x, y \in \Re\}$. A relation, R, is an $n-$ariry relation on $\prod_{i=1}^{n} A_i$ if R is a subset of $\prod_{i=1}^{n} A_i$. If $R = \emptyset$, then we say R is the *empty relation.* If $R = \prod_{i=1}^{n} A_i$, then we say R is the *universal relation.* If $n = 1$, then R is a *unary relation.* If $n = 2$, then R is a *binary relation.* If R is a binary relation on A, then $R \subset A \times A$. Let P be a predicate. Define P as $P < a_1, a_2, a_3, ..., a_n >$ is true iff $< a_1, a_2, ..., a_n > \in R$.

Example: Let A = natural numbers = $\{0, 1, 2, ...\}$. Let $P(x, y)$ mean $x < y$. P corresponds to a binary relation on A. $R = \{< x, y > | x < y\}$.

Some notation: $< a, b > \in R$ is donoted by $a\ R\ b$. Read page 124 and the top of page 125 in the textbook. There are 4 examples. Define $<$ (less-than relation). Basis: $0 < 1$. Induction: if $x < y$, then $x < y + 1$.

$x + 1 < y + 1$.

R is a binary relation on set A if $R \subset A \times A$. $\{< x, y > | x, y \in A\}$.

1.3.1 Graph Theory

A *directed graph (digraph)* is an ordered pair of the form $D =< A, R >$ where A is a set and R is a binary relation on A. $R \subset A \times A$. Elements of A are the *nodes* or *vertices* of the graph. Elements of R are the *edges* or *arcs* or *lines* of the graph. We will assume that A is finite. If $< x, y > \in R$, then we write $x\ R\ y$. This will mean that there is an arrow from x to y in the graph.

Example: $A = \{a, b, c\}$. $R = \{< a, b >, < b, c >, < c, c >\}$. $G :< A, R >$ is a graph.

To represent a graph in a computer:

1. Incidence matrix

	a	b	c
a	0	1	0
b	0	0	1
c	0	0	1

   This representation takes alot of space.

2. Adjacency list

An *edge* orginates at a and *terminates* at b. $A = \{a, b, c\}$. $D =< A, R >$. $R \subset A \times A$. $R = \{< a, b >, < a, c >, < b, a >, < b, c >, < c, c >\}$. Let $D =< A, R >$ be a directed graph with $a, b \in A$. An *undirected path* P from a to b is a finite sequence of verticies such that $P =< c_0, c_1, c_2, ..., c_n >$ such that 3 things are true:

1. $c_0 = a$.
2. $c_n = b$.
3. Either $c_i\ R\ c_{i+1}$ or $c_{i+1}\ R\ c_i, \forall 0 \leq i \leq n$. The latter is not in directed graphs. The path from b to c for undirected graphs is $< b, c >, < b, a, c >, < b, a, b, c, c >$. The path from c to b is undirected.

If P is a directed path from a to b then:

1. Vertex a is the initial vertex. Vertex b is the *terminal vertex.*
2. The length of the path is n edges.
3. If all the verticies of P are distinct except possibly c_0 and c_n, then P is a *simple* or *cordless path.*
4. If $c_0 = c_n$, then P is a cycle.

Digraph $D =< A, R >$ is *strongly connected* if for all verticies, $\forall a, b \in A$, there is a directed path from a to b and from b to a. D is *connected* if $\forall a, b \in A$ there is an undirected path from a to b. D is *disconnected* if there exist verticies $a, b \in A$ such that there is no undirected path between a and b.

Example: See Figure 1.15.

D is *complete over* A if $R = A \times A$. See Figure 1.16.

Let R be a binary relation on set A. $R \subset A \times A$. Then,

1. R is *reflexive* if $x\ R\ x\ \ \forall x \in A$. Loops.

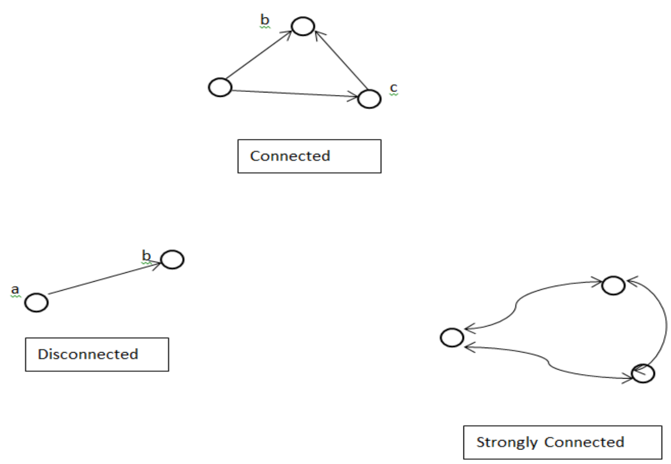

Figure 1.15: Diagram of a disconnected, strongly connected, and connected graphs.

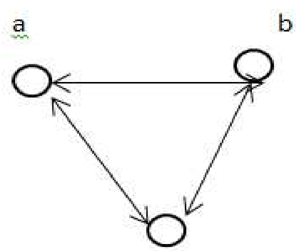

Figure 1.16: Diagram of a complete graph.

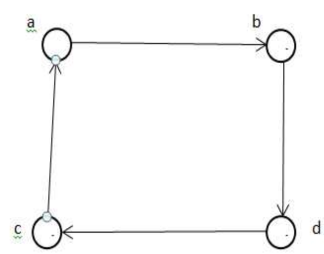

Figure 1.17: Diagram A for problem 2 on page 130 in the textbook.

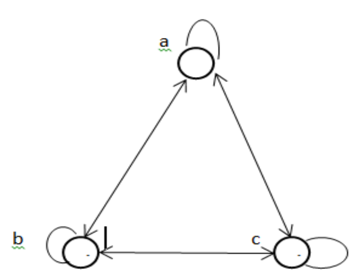

Figure 1.18: Diagram B for problem 2 on page 130 in the textbook.

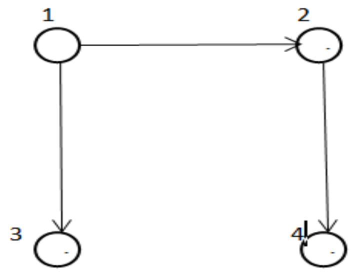

Figure 1.19: Diagram of the solution to homework question 3a on page 130 in the textbook.

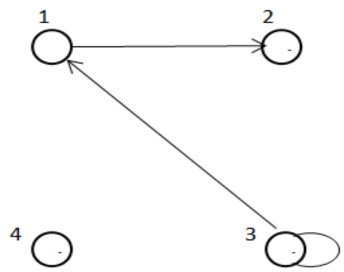

Figure 1.20: Diagram of the solution to homework question 3b on page 130 in the textbook.

2. R is *irreflexive* if $x \not R\ x \ \forall x \in A$. No loops.
3. R is *symmetric* if $x\ R\ y \Rightarrow y\ R\ x \forall x, y \in A$. 2 edges.
4. R is *antisymmetric* if $(x\ R\ y \wedge y\ R\ x) \Rightarrow (x = y) \forall x, y \in A$. No double edges.
5. R is *transitive* if $(x\ R\ y \wedge y\ R\ z) \Rightarrow x\ R\ z \forall x, y, z \in A$.

Do problems on page 130, #1, 2a, b, c, 3, 4, 5, 6.

1.3.2 Homework and Answers

Problems on page 130 in the textbook. #1, 2a, b, c, 3, 4, 5, 6.

1. Let $A = \{0, 1, 2, 3, 4\}$. For each of the predicates given below, specify the set of n-tuples in the n-ary relation over A which corresponds to the predicate. For parts (d) - (f), draw the diagram which represents the relation.

a. $P(x) \Leftrightarrow x \leq 1$. Solution: $R = \{< 0 >, < 1 >\}$.

b. $P(x) \Leftrightarrow 3 > 2$. Solution: $\{< 0 >, < 1 >, < 2 >, < 3 >, < 4 >\}$.

c. $P(x) \Leftrightarrow 2 > 3$. Solution: Always false $\emptyset$.

e. $P(x, y) \Leftrightarrow \exists k[x = ky \wedge k < 2]$. Solution: $K = 0, 1$. $R = \{< 0, 0 >, < 0, 2 >, < 0, 3 >, < 0, 4 >, < 1, 1 >, < 2, 2 >, < 3, 3 >, < 4, 4 >\}$.

2. For the following digraphs A and B in Figures 1.17 and 1.18.

a. Find all simple paths from node a to node c. Give the path lengths. Solution: Graph A. $< a, b, d, c >$. $n = 3$. Graph B $\{< a, c >\}$, $\{< a, b >, < b, c >\}$.

b. Find the indegree and outdegree of each node. Solution: Graph A. Indegree a 1, b 1, and c 1. Outdegree a 1, b 1, and c 1. Graph B. Indegree a 3, b 3, and c 3. Outdegree a 3, b 3, and c 3.

c. Find all simple cycles with initial and terminal node a. Solution: Graph $A : < a, bd, c, a >, < a >$. Graph $B : \{< a, b, c, a >\}\ \{< a, c, b, a >\}$.

3. For each of the following, sketch a digraph of the given binary relation on A. State whether the digraph is disconnected, connected, or strongly connected and state how many components the digraph has.

a. $[< 1, 2 >, < 1, 3 >, < 2, 4 >]$ where $A = \{1, 2, 3, 4\}$. Solution: Connected. See Figure 1.19.

b. $[< 1, 2 >, < 3, 1 >, < 3, 3 >]$ where $A = \{1, 2, 3, 4\}$. Solution: Disconnected. See Figure 1.20.

c. $[< x, y > |0 \leq x < y \leq 3]$ where $A = \{0, 1, 2, 3, 4\}$. Solution: Disconnected.

e. $[< x, y > |0 \leq x - y < 3]$ where $A = \{0, 1, 2, 3, 4\}$. Solution: $R = \{< 0, 0 >, < 1, 0 >, < 1, 1 >, < 2, 0 >, < 2, 1 >, < 2, 3 >, < 3, 1 >, < 3, 2 >, < 3, 3 >, < 4, 2 >, < 4, 3 >, < 4, 4 >\}$.

4. Construct the incidence matrix for the following binary relation on $[0, 1, 2, 3, 4, 5, 6] : \{< x, y > |x < y \vee x \text{ is prime } \}$. Solution: Connected.

1	2	3	4	5	6	7	8
0	0	1	1	1	1	1	1
1	0	0	1	1	1	1	1
2	1	1	1	1	1	1	1
3	1	1	1	1	1	1	1
4	0	0	0	0	0	1	1
5	1	1	1	1	1	1	1
4	0	0	0	0	0	0	0

5. For each of the following, give an inductive definition for the relation R on N. In each case, use your definition to show $x \in R$.

a. $R = \{< a, b > |a \geq b\}; x =< 3, 1 >$. Solution: Basis: $0 \geq 0$ or $< 0, 0 >\in R$ or $0\ R\ 0$. Induction: if $x \geq y$, then $x + 1 \geq y$ and $x + 1 \geq y + 1$. For example, prove that $5 \geq 3$.
$0 \geq 0$ basis
$1 \geq 0$
$2 \geq 0$
$3 \geq 1$
$4 \geq 2$
$5 \geq 3$.

b. $R = \{< a, b > |a = 2b\}; x =< 6, 3 >$. Solution: Basis: $< 0, 0 >\in R$. Induction: if $< x, y >\in R$, then $< x + 2, y + 1 >\in R$.

c. $R = \{< a, b, c > |a + b = c\}; x =< 1, 1, 2 >$. Solution: Basis: $< 0, 0, 0 >\in R$. Induction: If $< x, y, z >\in R$ then $< x + 1, y, z + 1 >\in R$. If $< x, y, z >\in R$ then $< x, y + 1, z + 1 >\in R$. Show that $< 2, 3, 5 >\in R$.
$< 0, 0, 0 >\in R$
$< 1, 0, 1 >\in R$
$< 2, 0, 2 >\in R$
$< 2, 1, 3 >\in R$
$< 2, 2, 4 >\in R$
$< 2, 3, 5 >\in R$.

6. Let $A = \{1, 2, 3\}$.

a. List the unary relation on A. Solution: If R is a unary relation on A, then $R \subset A$. $R = \emptyset$. $R = \{<1>, <2>, <3>\}$. $R = \{<1>\}, \{<2>\}, \{<3>\}, \{<1,2>\}, \{<1,3>\}, \{<2,3>\}$.

b. How many binary relations are there on A? Solution: $R \subset A \times A$ is a binary relation. $A \times A$ has 9 elements. $\therefore 2^9$ subsets $= 512$.

1.3.3 Homework and Answers

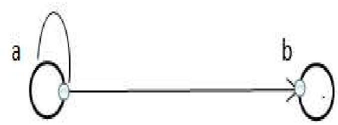

Figure 1.21: Diagram to homework question 1a on page 147 in the textbook.

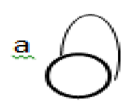

Figure 1.22: Diagram to homework question 1b on page 147 in the textbook.

Page 147 and 148 in the textbook.

1. List the properties defined in Definition 3.3.1 which hold for the relations represented by the following graphs.

a. See Figure 1.21. Solution: Not reflexive. Not irreflexive. Not symmetric. Antisymmetric. Transitive.

b. See Figure 1.22. Solution: Relfexive. Not irreflexive. Symmetric. Not antisymmetric. Transitive.

3. Consider the set of integers I. Fill in the following table with Yes and No according to whether the relation possesses the property. The notation $\emptyset$ denotes the empty set, $I \times I$ is the universal relation, and D denotes "divides with an integer quotient" (e.g. $4D8$ but $4\not{D}7$). Solution: $D : R = \{<x, y> | x$ divides $y\}$. For example, $<4, 8> \in R$.

$I \times I$	$\leq$	D
Reflective	Reflexive	Not reflexive
Not Irreflective	Not Irreflective	Not Irreflective
Symmetric	Not symmetric	No
Not antisymmetric	Antisymmetric	No
Transitive	Transitive	Yes

1.3.4 Composition of Relations

Let R_1 be a relation from A to B. $R_1 \subset A \times B$. Let R_2 be a relation from B to C. $R_2 \subset B \times C$. Then, the *composite relation* from A to C is denoted by $R_1 \cdot R_2$ or R_1R_2 and is given by $R_1R_2 = \{<a, c> | a \in A \wedge c \in C \wedge \exists b[b \in B \wedge <a, b> \in R_1 \wedge <b, c> \in R_2]\}$.

Example: $A = \{0, 1, 2\}$. $B = \{a, b, c\}$. $C = \{y, z\}$. $R_1 = \{<0, a>, <1, b>, <1, c>, <2, b>\}$. $R_2 = \{<a, 2>, <b, y>, <b, z>, <c, y>\}$. $R_1R_2 = \{<0, z>, <1, y>, <1, z>, <2, y>, <2, z>\}$. R_2R_1 is impossible.

If $R_1 \subset A \times B \wedge R_1 \subset B \times C$ then $R_1R_2 \subset A \times C$. $R_1R_2 = \{< a, c > | a \in A, c \in C, \exists b[b \in B \wedge < a, b > \in R_1 \wedge < b, c > \in R_2]\}$. Let R be a binary relation on set A. Then, the n^{th} *power of* R is denoted by R^n, is defined by

1. $R^0 = \{< x, x > | x \in A\}$ i.e. R^0 means "=."
2. $R^{n+1} = R^n \cdot R$.

Example: $A = \{a, b, c\}$. $R = \{< a, b >, < a, c >, < b, b >, < c, a >\}$. $R^0 = \{< a, a >, < b, b >, < c, c >\}$. $R^1 = R^0R = \{< a, b >, < a, c >, < b, b >, < c, a >\}$. $R^2 = R^1R = \{< a, b >, < a, a >, < c, b >, < c, c >, < b, b >\}$. $R^3 = R^2R = \{< a, b >, < a, c >, < b, b >, < c, b >, < c, a >\}$.

1.3.5 Closure Operations on Relations

Let R be a binary relation on set A. Then, the *reflexive closure* of R, $r(R)$, is the relation R' such that:

1. R' is reflexive.
2. R' is a super-set of R i.e. $R' \supset R$.
3. R' is the smallest relation which satisfies (1) and (2).

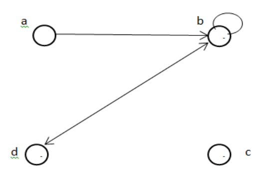

Figure 1.23: Diagram illustrating an example of adding arc to show the different relations.

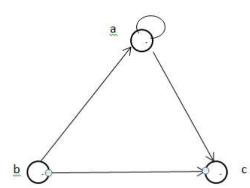

Figure 1.24: Diagram illustrating an example of reflexive, antisymmetric, transitive, and partial order.

Example: $A = \{a, b, c, d\}$. $R = \{< a, b >, < b, b >, < b, d >, < c, c >, < d, a >\}$. R is not reflexive. $R' = r(R) = \{< a, b >, < b, b >, < b, d >, < c, c >, < d, a >, < a, a >, < d, d >\}$.

Let E be the binary relation of equality on any set A i.e. $E = \{< x, x > | x \in A\}$. Notice that $r(R) = R \cup E$ by a computer.

Example: $A = \{a, b, c, d\}$. $R = \{< a, a >, < a, c >, < b, c >, < d, b >, < d, d >\}$. R is not symmetric. $A\ R\ c$ but $c \not R\ a$. $S(R) = \{< a, a >, < a, c >, < b, c >, < d, b >, < d, d >, < c, a >, < c, b >, b, d >\}$.

Let R be a binary relation on A. Then, R^c is called the *converse* of R and is given by $R^c = \{< y, x > | < x, y > \in R\}$. Result: $S(R) = R \cup R^c$ by a computer. Another result: R is symmetric iff $R = R^c$.

Example: $A = \{a, b, c\}$. $R = \{< a, b >, < b, a >, < a, c >\}$. R is not transitive. $t(R) = \{< a, b >< b, a >, < a, c >, < a, a >, < b, c >, < b, b >\}$. Note that $t(R) = R \cup R^n$.

Example: Consider Figure 1.23. $A = \{a, b, c, d\}$. Add $< a, a >, < c, c >, < d, d >$ to make it reflexive. Add $< b, c >$ to make it symmetric. Add $< a, d >, < d, a >$ to make it transitive.

Page 161 in the textbook, do problem 1.

Let R be a binary relation on set A. Then, R is a *partial order* if R is reflexive, antisymmetric, and transitive. The digraph $< A, R >$ is called a *partially ordered set* or *poset*. If R is a partial order on A then we write $a \leq b$, when $a \; R \; b$.

Example: "$\leq$" on integers is a partial order.

Example: "$\subset$" on the power $P(A)$ is a partial order. Let $T \in P(A)$. $T \subset T \Rightarrow$ reflexive. $T, S, R \in P(A)$. $T \subset S \wedge S \subset T \Rightarrow S = T \Rightarrow$ antisymmetric. $T \subset S \wedge S \subset R \Rightarrow T \subset R \Rightarrow$ transitive. See Figure 1.24

In a poset diagram, all loops are omitted; all edges implied by the transitive property are omitted; and all arrows are omitted. Let R be a binary relation on set A. R is a *quasi order* if R is transitive and irreflexive. Note it will also be antisymmetric. Does $(x \; R \; y \wedge y \; R \; x) \Rightarrow x = y$? If $x \; R \; y \wedge y \; R \; x$ then $x \; R \; x$ (transitive property) which is a contradiction by being irreflexive. Let $E = \{< x, x > | x \in A\}$. Results:

1. If R is a quasi-order then $R \cup E$ must be a partial order.
2. If R is a partial order then $R - E$ is quasi-order.

Partial order ($\leq$) on set A is a *linear order* if $a \leq b$ or $b \leq a, \forall a, b \in A$. The digraph $< A, R >$ is called a *linear ordered set.*

Example: "$\leq$" on I is a linear order.

Example: $A = \{a, b\}$. $P(A) = \{emptyset\}, \{a, b\}, \{a\}, \{b\}$. $R \sim' C'$. Not linear order.

If $< A, \leq >$ is a poset and if $B \subset A$, then:

1. $b \in B$ is a *greatest element* of B if $b' \leq b \forall b' \in B$.
2. $b \in B$ is a *least element* of B if $b \leq b' \forall b' \in B$.

Let R be a binary relation on A. Then R is a *well order* if R is a linear order and every non-empty subset of A has a least element. $< A, R >$ is called a *well ordered* set.

Example: "$\leq$" on I but is well ordered on N. It is a linear order.

On page 175 in the textbook, do problems 1 and 3.

1.3.6 Homework and Answers

Page 153 of the textbook, Section 3.4

1. Let R_1 and R_2 be relations on a set $A = \{a, b, c, d\}$ where $R_1 = \{< a, a >, < a, b >, b, d >\}$ and $R_2 = \{< a, d >, < b, c >, < b, d >, < c, b >\}$. Find R_1, R_2, $R_2 R_1$, R_1^1, and R_2^2. Solution: $R_1^2 = R_1^1 \cdot R_1 = \{< a, a >, < a, b >, < a, d >\}$.

9. Let R_1 and R_2 be arbitrary relations on a set A. Prove or disprove the following assertions.

a. If R_1 and R_2 are reflective, then R_1R_2 is reflective. Solution: True. b-e is False. R_1 is reflexive $\Rightarrow < x, x > \in R, \forall x \in A$. R_2 is reflexive $\Rightarrow < x, x > \in R_2 \forall x \in A$. $R_1R_2 < x, x > \forall x \in A$.

b. If R_1 and R_2 are irreflective, then R_1R_2 is irreflective. Solution: False. Find a counter example — one that is reflexive. $A = \{a, b, c\}$. $R_1 = \{< a, b >, < b, c >, < c, a >\}$. $R_2 = \{< b, a >, < c, b >, < b, c >\}$. $R_1 \cdot R_2 = \{< a, a >, < a, c >, < b, b >\}$. $\therefore R_1R_2$ is not irreflexive.

1.3.7 Homework and Answers

Page 161 of the textbook, Section 3.5

Figure 1.25: Diagram for problem 1b on page 161 in the textbook.

1b. Find the reflective, symmetric, and transitive closures of each of the graph in Figure 1.25. Solution: Reflexive $\{< b, b >\}$. Symmetric $\{< b, a >\}$. Already transitive.

1.3.8 Homework and Answers

Page 175, problems 1 and 3.

Figure 1.26: Diagram for problem 3a on page 175 in the textbook.

Figure 1.27: Diagram for problem 3b on page 175 in the textbook.

1. Fill in the following table describing the characteristics of the given ordered sets.

Figure 1.28: Diagram for problem 3c on page 175 in the textbook.

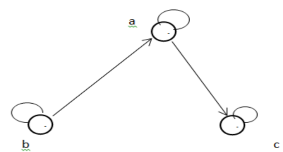

Figure 1.29: Diagram for problem 3d on page 175 in the textbook.

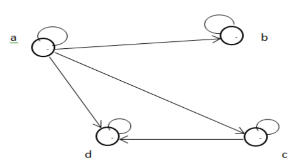

Figure 1.30: Diagram for problem 3e on page 175 in the textbook.

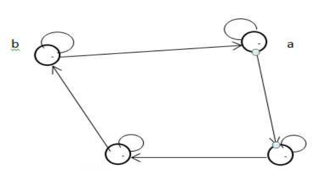

Figure 1.31: Diagram for problem 3f on page 175 in the textbook.

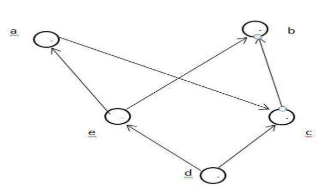

Figure 1.32: Diagram for problem 3g on page 175 in the textbook.

	Quasi Ordered	Partial Ordered	Linear Ordered	Well Ordered
$< N, <>$	Yes	No	No	No
$< N, \leq>$	No	Yes	Yes	Yes
$< I, \leq>$	No	Yes	Yes	No
$< R, \leq>$	No	Yes	Yes	No
$< P(N)$, proper containment $>$	Yes	No	No	No
$< P(N), \subset>$	No	Yes	No	No
$< P([a]), \subset>$	No	Yes	Yes	Yes
$< P([\emptyset]), \subset>$	No	Yes	Yes	Yes

3. State which of the following digraphs represent a quasi-order; a poset; a linearly ordered set; a well ordered set;

a. See Figure 1.26. Solution: Partial, not linear, not well.

b. See Figure 1.27. Solution: Partial, linear, well.

c. See Figure 1.28. Solution: No order. Symmetric.

d. See Figure 1.29. Solution: No order. Not transitive.

e. See Figure 1.30. Solution: Partial. Not linear $< b, d >, < b, c >$. Not well.

f. See Figure 1.31. Solution: Not partial — not transitive. Not linear, well quasi.

g. See Figure 1.32. Solution: No orders. Not reflexive or transitive.

The final exam will be Wednesday, December 9 from 1:00 to 2:00pm. It will cover Section 3.3 properties of binary relations; Section 3.4 Composition; also take powers of relations; Section 3.5 reflexive, symmetry, transitive closures of binary relation; Section 3.6 order relations. Office hours are Friday 10-12, Tues 10-12 and Weds 12-1.

1.3.9 Quiz 4

November 2, 1987

1. Using induction, prove the following $\sum_{i=1}^{n} i^3 = \left[\frac{n(n+1)}{2}\right]^2$. Solution: basis, let $n = 1$. Then $\sum_{i=1}^{1} i^3 = \left[\frac{1(1+1)}{2}\right]^2 = 1^3 = 1^2 = 1 = 1$. Induction: assume

$$\sum_{i=1}^{n} i^3 = \left[\frac{n(n+1)}{2}\right]^2 \text{ is true.}$$

Show

$$\sum_{i=1}^{n+1} i^3 = \left[\frac{(n+1)(n+2)}{2}\right]^2$$

is true.

$$\sum_{i=1}^{n+1} i^3 = \sum_{i=1}^{n} i^3 + (n+1)^3 =$$

$$\left[\frac{n(n+1)}{2}\right]^2 + (n+1)^3 =$$

$$\left[\frac{n(n+1)}{2}\right]\left[\frac{n(n+1)}{2}\right] + [(n+1)(n+1)(n+1)] =$$

$$(n+1)^2\left[\frac{n^2}{4} + n + 1\right] =$$

$$(n+1)^2\left[\frac{n^2}{4} + \frac{4n}{4} + \frac{4}{4}\right] =$$

$$(n+1)^2\left[\frac{n+2}{2}\right]^2 =$$

$$\left[\frac{(n+1)(n+2)}{2}\right]^2.$$

2. Define a set S inductively as follows:

   (a) $1 \in S$.

   (b) If $x \in S$, then $x1 \in S$.
   If $x \in S$, then $0x \in S$.
   If $x \in S$ and $y \in S$, then $xy \in S$.
   Using this definition, verify that $1101 \in S$. Solution: Basis: 1. Step 2 induction: 01. Step 3 induction: 101. Step 4 induction: 1101.

3. Let $\Sigma = \{c, d\}$, $A = \{c, dd\}$, $B = \{\Lambda, cd, d\}$, and $C = \{d\}$. Find:

   (a) AB. $\{c, dd\}$, $\{\Lambda, cd, d\}$. $AB = \{c, ccd, cd, dd, ddcd, ddd\}$.

   (b) A^2. $\{c, dd\}$, $\{c, dd\}$. $A^2 = \{cc, cdd, ddc, dddd\}$.

   (c) C^*. $C^0 \cup C^1 \cup C^2 \cup \cdots \cup C^n$ where $C^0 = \{\Lambda\}$, $C^1 = \{d\}$, $C^2 = C^1C = \{dd\}$, $C^3 = C^2C^1 = \{dd\}\{d\} = \{ddd\}$, and so on.

1.3.10 Exam 3

November 18, 1987

1. Prove by induction that $\sum_{i=1}^{n} 2^{i-1} = 2^n - 1$. Solution:
   Basis: $\sum_{i=1}^{1} 2^{i-1} = 2^1 - 1 = 2^{1-1} = 2^1 - 1 = 2^0 = 1 = 1 = 1$.
   Induction: Assume $\sum_{i=1}^{n} 2^{i-1} = 2^n - 1$ is true. Then show $\sum_{i=1}^{n+1} 2^{i-1} = 2^{(n+1)} - 1$.
   $\sum_{i=1}^{n+1} 2^{i-1} = 2^n + \sum_{i=1}^{n} 2^{i-1}$.

2. Let $\Sigma = \{c, d, g\}$ be an alphabet, and let $A = \{cg, d\}$ and $B = \{\Lambda, c, gg\}$ be languages over Σ. List the elements in the following sets.

   (a) AB. $\{cg, d\}$, $\{\Lambda, c, gg\}$. Solution: $AB = \{cg, d, cgc, dc, cggg, dgg\}$.

   (b) B^2. $\{\Lambda, c, gg\}$, $\{\Lambda, c, gg\}$.n Solution: $B^2 = \{\Lambda, c, gg, cc, cgg, ggc, gggg\}$.

   (c) A^+. $\{A' \cup A^2 \cup A^3 \cup \cdots$. $A^1 = \{cg, d\}$. Solution: $A^2 = \{cg, cg, cgd, dcg, dd\}$. $A^+ = \{cg, d, cgcg, cgd, dcg, dd, ...\}$

3. Give an inductive definition of the binary relation on $N = \{0, 1, 2, ...\}$ where $R = \{< a, b > | b = 3a\}$. $\{< 0, 0 >, < 1, 3 >, < 2, 6 >, ...\}$. Basis: $< 0, 0 > \in R$. Induction: if $< x, y > \in R$ then $< x+1, y+3 > \in R$.

4. Sketch the digraph which corresponds to $A = \{3, 4, 5, 6, 7, 8\}$ and $R = \{< x, y > | 2 \leq x - y < 4\}$. $R = \{< 8, 5 >, < 8, 6 >, < 7, 4 >, < 7, 5 >, < 6, 3 >, < 6, 4 >, 5, 3 >\}$. See Figure 1.33.

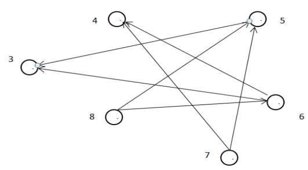

Figure 1.33: Digraph for problem 4 on Exam 3.

(a) Is the digraph connected, strongly connected, or disconnected? Connected. There are arrows to each vertex in the graph. It is not disconnected because there is an undirected path to each node.

(b) Give the incidence matrix for the digraph.

x/y	3	4	5	6	7	8
3	0	0	0	0	0	0
4	0	0	0	0	0	0
5	1	0	0	0	0	0
6	1	1	0	0	0	0
7	0	1	1	0	0	0
8	0	0	1	1	0	0

5. Let $A = \{x, y, z, w\}$. How many binary relations are there on A? Explain. Solution: $A \times A$ has $4 \times 4 = 16$ tuples. So, there are 2^{16} binary relations or subsets on A.

6. Indicate which of the properties listed are satisfied by the given digraph. For each property which is not satisfied, give an example to show it is not.

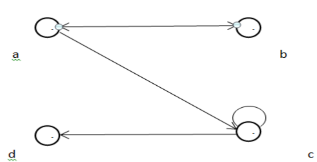

Figure 1.34: Digraph for problem 6a on Exam 3.

Figure 1.35: Digraph for problem 6b on Exam 3.

(a) See Figure 1.34. reflexive. No, a is not related to itself.
irreflexive. No, c is related to itself.
symmetric. No, $a\ R\ c$ but $c \not R\, a$.
antisymmetric. No, $a\ R\ b \wedge b\ R\ a$, but $a \neq b$.
transitive. No, $a\ R\ c \wedge c\ R\ d$, but $a \not R\, d$.

(b) See Figure 1.35. reflexive. Yes.
irreflexive. No, no node such that $x \not R\, x$.

symmetric. Yes.
antisymmetric. No, $a\ R\ c$ and $c\ R\ a$ but $c \neq a$.
transitive. Yes.

1.3.11 Quiz 5

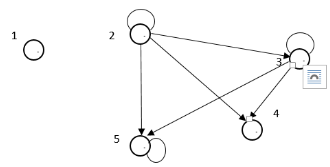

Figure 1.36: Digraph for problem 2 on Quiz 5.

1. Let $A = \{0, 1, 2, 3, 4\}$. Give the relation over A which corresponds to the predicate $P(x, y, z) \Leftrightarrow x+2y \geq z$. Solution: $R = \{< 0, 0, 0 >, < 0, 1, 2 >, < 0, 2, 4 >, < 1, 0, 1 >, < 1, 1, 3 >, < 2, 0, 2 >, < 2, 1, 4 >, < 3, 0, 3 >, < 4, 0, 4 >\}$. The L. J. Randall's comment is "there are many others."

2. Let $A = \{1, 2, 3, 4, 5\}$ and let R be the binary relation on A defined by $R = \{< x, y > | x$ is prime and $x \leq y\}$. Sketch the digraph which corresponds to $< A, R >$. Solution: See Figure 1.36.

3. Give an inductive definition of the relation of $>$ on $N = \{0, 1, 2, ...\}$. Solution: basis $< 1, 0 > \in R$. Induction: if $< x, y > \in R$, then a) $x + 1 > y$, and b) $x + 1 > y + 1$.

   (a) Use your definition to verify that $6 > 4$. Solution: basis $< 1, 0 >$. Induction
   $< 2, 1 >$
   $< 3, 2 >$
   $< 4, 3 >$
   $< 5, 4 >$
   $< 6, 4 >$

Chapter 2

Theory of Formal Languages

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CS 390/590
Course Outline, Summer 1988
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Course Description: This is an introduction to theoretical computer science. Topics covered will include Turing machines, foundational programming languages, computable functions, context-free grammars for formal languages, and finite automata.

Prerequisites: CS 281

Text: *Elementary Computability, Formal Languages, and Automata,* by Robert McNaughton.

Grading for 390: Your grade will be based on three tests, including the final. Each test will be 33.33% of your grade.

Make-up tests: A test may be made up only if I am contacted within 24 hours after the test is given and if the reason for absence is legitimate.

Attendance policy: Students are expected to attend class. A student who must miss class is expected to obtain the assignment and be prepared for the next class meeting.

Honor code: All students are expected to abide by the ODU Honor Code. An honor pledge will be required on all work which is to be graded.

2.1 Overview of the Course

This section gives an overview of the course. There are 3 main topics:

1. Computability — The study of what is computable and what is not; what problems can be solved using *algorithms.*
2. Formal languages — Special languages like programming languages or symbolic logic which have strict rules governing them.
3. Automata — Idealized computational models such as computers of which there is no physical instance.

The *theory of computability* is a study of problems which are solvable by algorithms and of problems which are not solvable. A *problem* is a class of questions. Each question in the class is an *instant* of the problem.

Example: Problem: What is the value of $2x + 1$ where x is some integer?

Example: Instance: What is the value of $2x + 1$ when $x = 5$?

We will assume that all questions (and answers) must be expressed in some written language like English or a programming language. We also assume that it is possible to determine whether an answer to a problem is correct or not. There are two math problem types:

1. Determine the value of a function for given values for its arguments. For example, if $f(x) = 2x + 1$, find $f(5)$.
2. Decidable problems. Problems requiring yes/no answers. For example, is $x = 3$ a solution to the equation $x^2 + 1 = 12$?

An *algorithm* for a problem is an organized set of commands for answering on demand any question that is an instance of the problem subject to the following:

1. The algorithm is written as a finite expression A, in some language.
2. Exactly which question is answered by executing the algorithm is determined by setting the *inputs* before execution begins.
3. Execution of the algorithm is a step-by-step process where the total result of the action during any one step is simple.
4. The action at each step and all results of this action are strictly determined by expression A, by the inputs, and by the results of the previous steps.
5. Upon termination, the answer to the question is a clearly specified part (the output) of the result of execution.
6. Whatever the input values, execution will terminate after a *finite* number of steps.

A *procedure* for a problem is an organized set of commands which satisfy conditions (1) thru (5) of the definition of the algorithm i.e. there may be inputs such that the procedure does not terminate after a finite number of steps. A future result will tell us that there is no method (or algorithm) for determining whether a procedure will always halt or even whether it will halt for a particular set of inputs. This is called the *halting problem.* A *non-deterministic procedure* is an organized set which satisfy conditions (1), (2), (3) and (5). A problem is *solvable* if there is an algorithm for it. Otherwise, it is *non-solvable.* A *decision procedure* is an algorithm for a class of questions for which all answers are either "yes" or "no." A problem is *decidable* if it has a decision procedure. It is *un-decidable* otherwise. Some examples of algorithms include the Euclidean algorithm for finding the greatest common divisor of two natural numbers; and the Labyrinth algorithm for determining whether a particular object is in a labyrinth.

We will represent the labyrinth by a graph. A *graph* is a ordered pair (N, E) where N is a finite set of *nodes* and E is a finite set of *edges,* each of which connects two distinct nodes. See Figure **??**. A *walk* from N_0 to

N_n is a sequence where $n \geq 0$ and E_i connects nodes N_{j-1} and N_j.

Example: $A, e_1, B, e_3, C, e_4, D$ is a walk from A to D.

A *path* from N_0 to N_n is a walk $N_0, E_1, N_1, E_2, ..., E_n, N_n$ where $N_i \neq N_j$ where $i \neq j$. All nodes are distinct in a path. A graph is *connected* if for any two nodes, there is a path between them. Some assumptions for the labyrinth problem include:

1. The graph representing the labyrinth must be connected.
2. There is an origin node labeled A.
3. One of the edges from A is named the *leading edge.*
4. If there is a target node in the labyrinth, it is labeled T.
5. Initially, no nodes or edges are colored.
6. Edges can be colored and re-colored using the colors yellow and red.

The labyrinth problem: beginning at A, travel through the graph and determine whether or not there is a node labeled T. Return to node A with the answer. See Figure **??**

2.2 Turing Machines

Alan Turing proposed Turing machines in a 1936 paper. The Turing machine, as discussed here, is a n example of a *deterministic finite state automaton.* The machine consists of a read/write head and infinite tape. The machine can assume a finite number of states and works with a finite character set. During a time cycle, the machine reads on a position on the tape and either halts or takes an action depending on what it reads and the state that it is in at the time of the read. There are at most four possible actions per time cycle:

1. Erase the symbol, just read.
2. Print a new symbol at the current position if there is no symbol already there.
3. Move one position left or right.
4. Change to a new state.

We will discuss how a Turing machine works by means of a *table* which gives all possible states, all possible characters which can be read, and the corresponding actions taken. Some notation: B represents a blank. No entry in the table means the machine halts in that situation. Execution begins at the first non-blank character. See Figure **??**.

R	Move one position to the right.
L	Move one position to the left.
$*$	Indicates start of new number.
q_i	State change.

Example: Consider the input $*//*///$. The output is $*/////$. It adds two numbers.

We will represent non-negative integers by using a unary number system.

$0 \to *$
$1 \to */$
$2 \to *//$
$3 \to *///$

When the input consists of more than one number, we write them consecutively on tape. See Figure 2.1.6 on page 28 in the textbook. Analysis:

1. The input is a string over the alphabet $\{b, c\}$.
2. An $*$ will be used to separate the input string from the copy.
3. The machine alphabet will consist of $\{b, c, *, y, z\}$.
4. As characters from the input string are copied, "b" will be changed to "y" and "c" will be changed to "z."
5. The "y's" and "z's" are changed back to "b's" and "c's" at the end.

Example: Input $\rightarrow c\ b\ b\ c$.

$$
\begin{array}{cccccccc}
 & \text{c} & \text{b} & \text{b} & \text{c} & * & \text{c} & \text{b} \\
 & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & & \\
 & q_1 & \rightarrow & \rightarrow & \rightarrow & \rightarrow & & \\
\uparrow & \uparrow & \uparrow & \uparrow & \uparrow & & & \\
\leftarrow & \leftarrow & \leftarrow & \leftarrow & q_2 & & & \\
 & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \\
 & q_3 & q_c & \rightarrow & \rightarrow & \rightarrow & \rightarrow & \\
\leftarrow & \leftarrow & \leftarrow & \leftarrow & \leftarrow & q_2 & & \\
 & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\
 & q_3 & & q_b & & & q_2 &
\end{array}
$$

Finish the table for homework.

Turing machines are often used to compute function values. Turing machine M computes function f with n non-negative integer arguments $i_1, i_2, ..., i_n$ if M begins with the sequence $i_1, i_2, ..., i_n$ as input and upon halting, contains *one number* on the tape which is $f(i_1, i_2, ..., i_n)$. Figure 2.1.8 in the textbook is not a function. It leaves two numbers on the output string. Figure 2.1.8 in the textbook analysis:

1. A copies the strokes of i into the positions immediately following the strokes of j.
2. As each stroke is copies, ..., etc.

Figure 2.1.9 in the textbook is multiplication. The input string $*//*/// \Rightarrow *//*///* \Rightarrow */B*///*/// \Rightarrow *BB*///*//////$.

Homework: On page 34 of the textbook, problems 1 thru 4, 8 thru 11. Skip Sections 2.2.1, 2.2.2, 2.2.3, and 2.2.4.

2.3 The Foundational Programming Languages

To study algorithms in terms of programs, we will develop two simplistic programming languages:

1. The Goto language.
2. The While language.

Both the Goto and While languages are *formal string languages.* The rules that govern them is very precise. To define each language, we do the following:

1. Enumerate the alphabet.
2. Define certain kinds of strings called *syntactic categories.*
3. Explain the meaning of each string in each syntactic category (semantics).

2.3.1 The Goto Language

The alphabet of the Goto language consists of 0-9, A, B, ..., Z (capitals only), :, ;, =, (,). The syntax categories are:

1. Numeral — a single digit or a string of digits which does not begin with zero.

2. Name — any string of letters and digits which begins with a letter.

3. Unlabeled command — there are 7 types.

   (a) Name := name — unlabeled variable assignment.
   (b) Name := numeral — unlabeled numerical assignment.
   (c) INCR(name) — unlabeled increment.
   (d) DECR(name) — unlabeled decrement.
   (e) GOTO name — unlabeled unconditional transfer.
   (f) If name = 0 GOTO name — unlabeled conditional transfer.
   (g) HALT — unlabeled halt.

4. Name — unlabeled command (label)

5. Program — a single command or a sequence of commands (labeled or unlabeled) seperated by semicolons. Blanks are not part of the syntax.

See Section 3.1.3 in the textbook for a discussion of parsing a program in the GOTO language. The semantics of the GOTO assumptions are:

1. The machine has unlimited storage.

2. All numbers are non-negative integers.

3. Before execution, each variable is assigned a storage location and input values are loaded into these locations.

See Section 3.2.1 in the textbook for a complete description of the meaning of each command.

Example: $DECR(x1)$ means subtract 1 from the storage location for $x1$, unless $x1$ is zero.

Notice the conditions which will cause the machine to halt. Know the three ways. A *time cycle* is the time during which the machine executes one command. A *run history* is a table showing each time cycle, the command executed, and the numbers in each storage location at the beginning and end of each time cycle. Consider Figure 3.2.1 on page 50 in the textbook which adds x, y and stores in z. Define a *proper program* in the Goto language as one satisfying:

1. For every label after a GOTO, there is exactly one labeled command in the program which has that label.

2. The last command is either a halt or an unconditional transfer. Avoid the default halt situation.

Homework, page 34, problems 1, 2,3, 4, 8, 9, 10, 11 in the textbook.

2.3.2 Homework and Answers

This is the assignment on page 34 in the textbook. Problems 1 thru 4, 8 thru 11.

These computations are similar to the copying machine of Section 2.1.3 in the textbook. In each case, design a Turing machine which, when given a string W over the alphabet $\{c, d\}$ will transform the tape into the output tape as indicated. The input string W is to be written on consecutive squares of an otherwise blank tape; and your machine is to begin in state q_1 on the leftmost nonblank square. Make sure that your machine computes correctly for every string W of length one or more over the alphabet $\{c, d\}$.

There is no restriction on how much tape you may use in the computation; or on which particular set of squares in reference to the input location the output string appears on. However, the output must appear exactly as specified, which may require that the machine "clean up" excess characters before halting. Nothing but the output should be on the output at the halt.

1. The output is the string W written backwards on consecutive squares. Solution:

State	B	c	d	z	$*$
q_1	$*q_3$	R	R		
q_2	q_4	L	L		Lq_3
q_3	Rq_5	zRq_c	zRq_d	L	L
q_c	cLq_2	R	R	R	R
q_d	dLq_2	R	R	R	R
q_4	Rq_5				
q_5				BR	BR

2. The output is a string written on consecutive squares with the same number of $c's$ and with the same number of $d's$. In other words, the output is the input string with the input characters put in alphabetical order. Solution:

1 [Place * at end
  2 [loop: find c;
    change to z — send to end;]
  restart]

3 [loop: find d;
  change to z — send to end;]

State	B	d	c	z	$*$
a_1	$*La_2$	R	R		
a_2	Ra_4	L	zRa_c	L	L
a_c	cLa_3	R	R	R	R
a_3	a_2	L	L	L	L
a_4		R		R	La_5
a_5	a_{10}	zRa_d		L	
a_d	dLa_6	R	R	R	R
a_6		L	L		La_7
a_7	Ra_8	zRa_d		L	
a_8				BR	BR

3. The output is the string W written on the tape with a single blank space between each pair of adjacent characters. Solution:

Comment	State	B	c	d	z	$/$	$*$
Initialize	a_1	a_2	R	R			
	a_2	$*La_3$					
Reset	a_3	Ra_4	L	L	L	L	L
Put c at end	a_4		zRa_c	zRa_d	R		La_5
	a_c	ca_{c2}	R	R		R	R
	a_{c2}		R/a_3				
	a_d	da_{d2}	R	R		R	R
	a_{d2}			R/a_3			
Clean-up	a_5	Ra_6			L	L	
	a_6		R	R	BR	BR	BR

4. The output is the string W (as written as input) followed without a blank by (1)*MORE.; if there are more $c's$ than $d's$ in W. (2) *EQUAL; if there are as many $c's$ as $d's$ in W, or (3) LESS; if there are fewer $c's$ than $d's$ in W. Solution:

State	B	c	d	x	y	$*$	Comment
a_1	a_2	R	R				
a_2	$*La_3$						
a_3	Ra_4	L	L			L	
a_4		a_5	a_5			B	empty string
a_5		xa_6	R	R	R	a_a	more $d's$
a_6	Ra_7	L	L	L	L		
a_7		R	ya_8	R	R	a_{11}	more or equal $c's$
a_8	Ra_5	L	L	L	L		
a_9			R	R	R	Ra_{10}	less $c's$
a_{10}	Less a_{14}						
a_{11}		R	a_{12}	R	R	Ra_{13}	
a_{12}	More a_{14}	R		R	R	R	more $c's$
a_{13}	Equal a_{14}						Equal $c's$
a_{14}	Ra_{15}	L	L	L	L	L	Clean-up
a_{15}				cR	dR		

Design Turing machines to compute the following functions according to the conventions laid down in Section 2.1.4 in the textbook.

8. Absolute difference:

$$|i_1 - i_2| = \begin{cases} i_1 - i_2, & \text{If } i_1 \geq i_2. \\ i_2 - i_1, & \text{If } i_1 < i_2. \end{cases}$$

Solution:

State	B	$/$	$*$	$\$$	α	x	Comment
a_1	a_2	R	R				
a_2	$\$La_3$						
a_3	B	L	$\alpha La_{3,5}$				
a_4		xRa_5	R		Ra_8	R	cancel /'s
a_5		R			Ra_6		
a_6		xa_7				R	
a_7		L	a_4	La_{11}	L	L	
a_8		xRa_9				R	$i_1 > i_2$
a_9	$/a_{10}$	R		R			
a_{10}		L		L		Ra_8	
a_{11}		L	a_{12}	L	L	L	
a_{12}		xRa_{15}	R	R	Ra_{13}	R	
a_{13}	$/a_{14}$	R		R		R	
a_{14}		a_{16}					
a_{15}	$/a_{11}$	R		R	R	R	$i_1 > i_2$
a_{16}		L	a_{17}	L	L	L	clean-up
a_{17}		R	BR	$*$	BR	BR	

9. $QU(i_1, i_2)$ equals to the quotient when i_1 is divided by i_2. This is sometimes written as $[i_1/i_2]$ or $\lfloor i_1/i_2 \rfloor$. The quotient is the greatest integer not greater than i_1/i_2. Solution: $QU(i_1, i_2)$. $\overbrace{*///////*//*/}^{\text{bb bb}}$. $\overbrace{*/////}^{\text{bbbbb}}\ bb\ \overbrace{*//}^{\text{bb}}*///$.

State	B	$*$	α	$/$	x	$\$$	Comment
a_1	$\$La_2$	R		R			Prep string
a_2		αa_3		L			
a_3		Ra_4	L	L			
a_4		a_{11}	Ra_5	R	R		
a_5				xLa_6	R	a_8	Division
a_6			La_7		L		
a_7		a_{11}		xRa_4	L		
a_8	$/La_9$			R		R	
a_9				L		La_{10}	
a_{10}			a_4		$/L$		Reset divisor
a_{11}		BR	BR		BR	$*a_{12}$	Clean-up
a_{12}							

10. $REM(i_1, i_2)\ *//\ \overbrace{///}^{\text{bbb}} * \overbrace{///}^{\text{bbb}} .\ \overbrace{*//}^{\text{bb}}\ bbb * \overbrace{///}^{\text{bbb}}$ where b = erase.

11. $MIN(x_1, ..., x_n)$ equals to the smallest value among $x_1, x_2, ..., x_n$. Your Turing machine should work for any value of $n \geq 2$. Solution: $MIN(x1, x2)$. $*\overbrace{///}^{\text{ccc}}//*\overbrace{//}^{\text{cc}}.*\overbrace{//}^{\text{cc}}*\overbrace{//}^{\text{cc}}///*\overbrace{//}^{\text{cc}}//*\overbrace{//}^{\text{cc}}///$ where c = erase.

State	B	/	x	*	\$	y	Comment
a_1	$\$La_2$	R	R				Prep string
a_2	Ra_3	L	L				
a_3				Ra_4			
a_4		xRa_5					Find min
a_5		Ra_6		a_7	a_7		
a_6				a_3			
a_7				La_8			
a_8			yL	a_9			Put min at end
a_9				R		xa_{10}	
a_{10}	$/a_{11}$	R	R	R	R	R	
a_{11}	a_{12}	L	L	L	L	a_9	
a_{12}	Ra_{13}						Clean-up
a_{13}		BR	BR	BR	a_{14}		
a_{14}					*		

2.3.3 The While Language

The alphabet is the same as the GOTO language plus the characters >, [,]. The syntactic categories are:

1. Numeral — a single digit or a string of digits which does not begin with zero.
2. Name — any string of letters and digits which begins with a letter.
3. Command — 7 types (unlabeled).
   (a) Variable assignment — := name is an unlabeled variable assignment. Level 0 command.
   (b) Numeric assignment — Name := numeral is an unlabeled numerical assignment. Level 0 command.
   (c) Increment — INCR(name) is an unlabeled increment. Level 0 command.
   (d) Decrement — DECR(name) is an unlabeled decrement. Level 0 command.
   (e) Unilateral conditional of level $i+1$ ($i \geq 0$) : If name $=0$ then [Program of level i]
   (f) Bilateral conditional of level $i+1$: If name $=0$ then [Program of level i] Else [Program of level k] where $i = \max(i,k)$.
   (g) While command of level $i+1$: While name >0 Do [Program of level i]

A program of level i is a command of level i or a sequence of commands of maximum level i separated by semicolons. Levels tell how deeply nested commands are. There are no labels in the While language. Halt is missing. Each command is executed in turn. The machine halts after the last command is executed. See Section 3.3.2 in the textbook for a description of how commands are executed. In Figure 3.3.1 on page 56 of the textbook, the second While is level 1; the first While is level 2; and Program is level 2. A While language program can easily be translated into the Goto language such that the two programs have identical flowcharts. It is not always possible to translate a Goto language program into the While language and have identical flowcharts.

Homework: page 57, problem 1 in the textbook.

2.3.4 Flowcharts

A *flowchart* is a *directed graph.* A directed graph is an ordered pair (N, A) where N is a finite set of nodes and A is a finite set of arcs or edges. Each arc goes from a node to a node (possibly the same node). A *walk* and a *path* are defined for a directed graph similar to the directions in Section 2.1. A *flowchart* is a directed graph whose nodes are circles, rectangles, and diamonds.

- Rectangle — represents a command.

- Circle — represents Begin, Halt.
- Diamond — represents a decision.

A flowchart represents a program. The language of flowcharts is a non-string formal language. Figure 3.4.1 on page 60 in the textbook is the sum of $x + y = z$. Figure 3.4.2 in the textbook is a schematic flowchart. It contains non-existent commands. Some programs may not always halt. Many functions are extremely difficult to compute. It may be hard to check that all possible situations eventually halt. Some math programs seek to find a number which satisfies a certain property without knowing whether such a number exists. Future results:

1. All computable functions can be expressed as programs in the Goto and While language.
2. There is no algorithm to tell whether a program in the Goto and While language will halt for a given input.

For homework, do problems 1, 2, 4, 5, 7, 8, 9, 10, 11, and 12 on page 64 in the textbook.

2.3.5 Homework and Answers

Page 57, problem 1 in the textbook.

1. Consider the following WHILE-language program of level 3 in which X and Y are inputs; Z is an output; and U is an auxiliary variable. Translate the program on page 58 in the textbook into a GOTO-language program, in executing which the machine will do the same things in order for each value of the inputs X and Y. Your program must have exactly the same variables, inputs, and outputs; and at the halt the value of the output must be the same. The program in this exercise computes the function $Z = f(X, Y)$ where $f(X, Y)$ is the sum of the positive terms in the sequence $2x, 2(x-3), 2(x-6), ..., 2(x-3(y-1)), (x-3y), (x-3y-1), (x-3y-2), ...$ For $Y = 0$, this sequence is $X, X-1, X-2, ...$ Solution:

```
  z:= 0
  INCR(y);
  same: If x = 0 then HALT;
  u := x;
  DECR(y);

  if y = 0 then GOTO loopif;
  DECR(x);
  DECR(x);
  DECR(x);
1 loop1: If u = 0 then GOTO same;
  DECR(u);
  INCR(z);
  INCR(z);
  GOTO loop1;

  loopif: DECR(x);
  loop2: if u = 0 then GOTO same;
  DECR(u);
  INCR(z);
  GOTO loop2;
```

2.3.6 Homework and Answers

Page 64, problems 1, 2, 4, 5, 7, 8, 9, 10, 11, and 12.

1. Give a run history in tabular form for the multiplication program in the GOTO language which was given for the flowchart of Figure 3.4.4, assuming that X, Y, W, and U are set at 3 and 2;1914, and 1939, respectfully. You will trace the multiplication of 3 by 2. Number the commands in the program 1 thru 9. Solution:

```
Time
Cycle  Line    x    y   W      U
---------------------------------
          \    3    2  1914   1939
  1       1 -----------------------
          /    -    -   0      -
          \
  2       2 -----------------------
          /
          \    -    -   -      -
  3       3 -----------------------
          /
          \    -    1   -      -
  4       4 -----------------------
          /
          \    -    -   -      3
  5       5 -----------------------
          /
          \    -    -   -      -
  6       6 -----------------------
          /
          \    -    -   -      2

and so on...
```

In each of the following, write a program to compute the function F that is indicated. Let $x1, X2, X3, ...$ and so on, be your input variables; or simply Xif there is only one; and let Y be your output variable, with auxiliary variables as you see fit. The values of your input variables may be destroyed in the working of your program. You may give your answer as a detailed flowchart, as a GOTO-language program, or as a WHILE-language program, as you choose.

2. $F(X1, X2)$ is the maximum of two values $X1, X2$. Solution:

1
y:= 0
loop: If x1 = 0 then GOTO bottom1;
DECR(x1);
if x2 = 0 then GOTO bottom2;
DECR(x2);
GOTO loop;
bottom1: y:= x1;
Halt;
bottom2: y:= x2;
Halt;

5. The given function is:

$$f(x1, x2) = \begin{cases} 0, & \text{If } X1 \leq X2. \\ X1 - X2, & \text{If } X1 > X2. \end{cases}$$

Solution:

1

```
if x1 = 0 then GOTO case3;
top: DECR(x1);
if x1 = 0 then GOTO case1;
DECR(x2);
if x2 = 0 then GOTO case2;
GOTO top;
case1: y:= x1;
DECR(x2);
if x2 = 0 then y:=0;
HALT;
case2: y:= x1;
HALT;
case3: y:= 0;
HALT;
```

7. The given function is:

$$f(x) = \begin{cases} X, & \text{If } X \text{ is divisible by 3.} \\ X - 1, & \text{If } X \text{ is not divisible by 3.} \end{cases}$$

Solution:

1

```
x1:= x;
top: DECR(x1);
if x1 = 0 then GOTO bottom2;
DECR(x1);
if x1 = 0 then GOTO bottom2;
DECR(x1);
if x1 = 0 then GOTO bottom;
GOTO top;
bottom2: y:= DECR(x);
HALT;
bottom: y:=x;
HALT;
```

8. The given function is:

$$f(x) = \begin{cases} 2X, & \text{If } X \text{ is even.} \\ 3X, & \text{If } X \text{ is odd.} \end{cases}$$

Solution:

1

```
x1:=x;
top: DECR(x1);
if x1 = 0 then GOTO x2;
DECR(x1);
if x1 = 0 then GOTO x3;
GOTO top;
x3: w:= 0; z:= 2;
outter: if z = 0 GOTO exit1;
DECR(z);
u:= x;
inner: if u = 0 GOTO outter;
DECR(u);
INCR(w);
GOTO inner;
exit1: HALT;
x2: w:= 0; z:= 3;
outter2: if z = 0 GOTO exit2;
DECR(z);
u:= x;
inner2: if u = 0 then GOTO outter2;
DECR(u);
INCR(w);
GOTO inner2;
exit2: HALT;
```

9. The given function is:

$$f(X1, X2) = \begin{cases} 0, & \text{If } X1 = X2. \\ 1, & \text{If } X1 \neq X2. \end{cases}$$

Solution:

1

```
top: DECR(x1);
DECR(x2);
if x1 = 0 then GOTO bottom;
if x2 = 0 then GOTO bottom2;
GOTO top;
bottom: if x2 = 0 then GOTO exityes;
y:= 1;
HALT;
exityes: y:= 0;
HALT;
bottom2: if x1 = 0 then GOTO exit2yes;
y:= 1;
HALT;
exit2yes: y:= 0;
HALT;
```

11. $F(X1, X2)$ is the quotient when $X1$ is divided by $X2 \neq 0$. $F(X1, X2) = 0$ if $X2 = 0$. See Figure 2.1 for the solution.

12. $F(X1, X2)$ is the remainder when $X1$ is divided by $X2 \neq 0$. $F(X1, X2) = X1$ if $X2 = 0$. See Figure 2.2 for the solution.

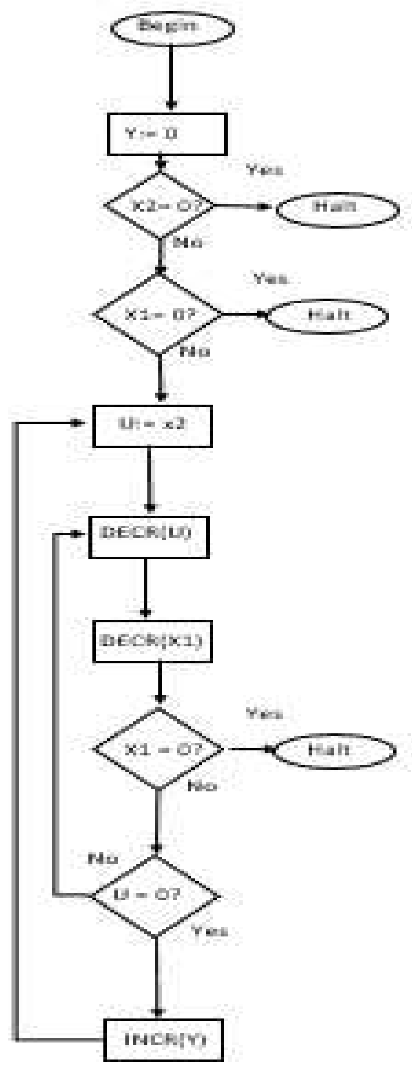


Figure 2.1: This figure shows the solution to problem 11 on page 65 in the textbook

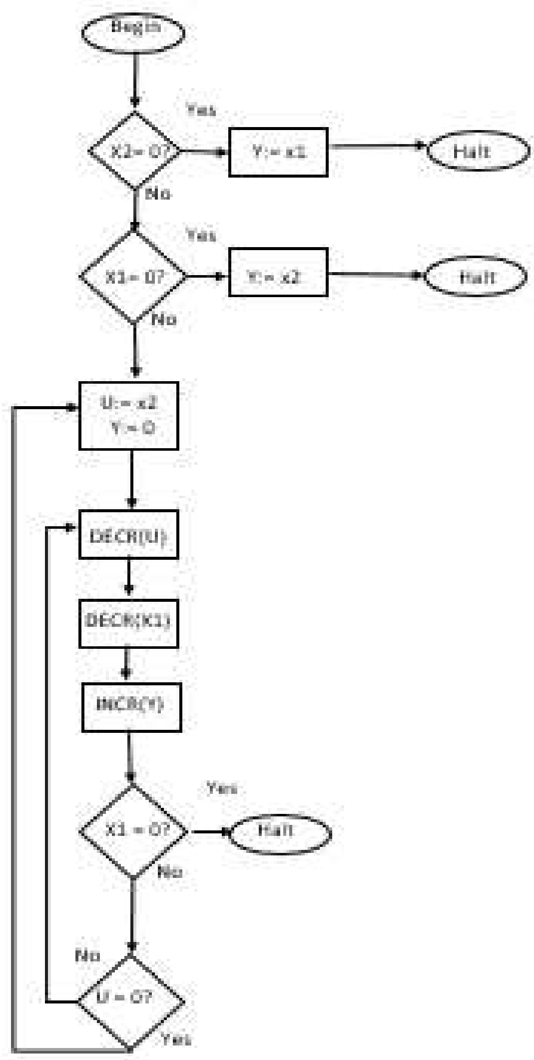


Figure 2.2: This figure shows the solution to problem 12 on page 65 in the textbook

2.3.7 Exam 1 and Answers

1. Explain the difference between an algorithm and a procedure. Solution: An algorithm always halts. A procedure may or may not halt. Procedures contain algorithms.

2. The Euclidean Algorithm produces an answer to the problem "find the greatest divisor of two positive integers x_1 and x_2."

   (a) Give an instance of this problem. Solution: $x_1 = 3$ and $x_2 = 6$. Find the GCD. The answer is 3.

   (b) Is this problem solvable or decidable? Explain. Solution: The GCD problem is solvable. It's not decidable because it does not return a yes / no answer. It is solvable because there is algorithm for it.

3. An algorithm must be deterministic. Explain what this means. Solution: Given the same set of inputs for each execution of the same algorithm, the algorithm will execute the same steps in the same order every time. To be deterministic means that the result of a step depends on expression A (the algorithm), the inputs and the results of previous steps.

4. Design a Turing machine which takes as input a non-empty string W over the alphabet $\{a, b\}$ and which produces as output string W with the first and last characters interchanged. For example, if the input is abbab, then the output is bbbaa. Give a short description of each state of your machine. Be sure to cover special cases such as strings of length one. Solution:

State	B	a	b	z	$*$	
a_1	a_2	R	R			prepare string
a_2	$*La_3$					
a_3	Ra_6	L	zRa	L	L	find all $b's$
a_4	a_5	R	R	R	R	
a_5	bL		L		a_3	
a_6		zRa_7		R	a_{10}	find all $a's$
a_7	a_8	R	R	R	R	
a_8	aLa_9					
a_9	Ra_6	L	L	L	L	
a_{10}				BL	BL	erase input

5. Write a GOTO language program to compute the function $F(X1, X2) = MIN(X1, X2)$. Use Y as your output variable.

```
z1:= x1;
z2:= x2;
top: DECR(z1);
If z1 = 0 Then GOTO minx1;
DECR(z2);
If z2 = 0 then GOTO minz2;
GOTO top;
minx1: y:= x1;
HALT;
minx2: y:= x2;
HALT;
```

6. Describe the difference between a total function and a partial function. Solution: A total function always returns one value for n-tuples; otherwise it is a partial function.

   (a) Give an example of a total function. Solution: addition.

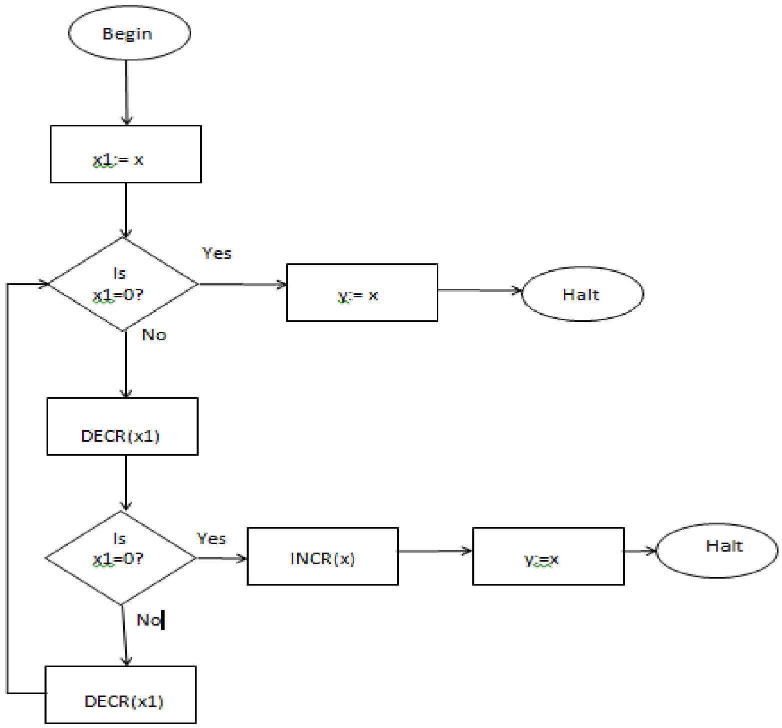


Figure 2.3: This figure shows the flowchart for problem 8 on Exam 1

(b) Give an example of a partial function. Solution: square root.

7. Write a DO-TIMES program to compute the function:

$$f(x_1, x_2) = \begin{cases} 0, & \text{If } x_1 \leq x_2. \\ x_1 - x_2, & \text{If } x_1 > x_2. \end{cases}$$

Use y as your output variable.

```
1 [ z1:= x1:
    z2:= x2;
    DO z1 TIMES
    [DECR(z1);
    DECR(z2);
    If z2 = 0 Then [y:= z1]
    Else y:= 0]
```

8. Give either a WHILE language program or a detailed flowchart to compute the function:

$$f(x) = \begin{cases} x, & \text{If } x \text{ is even.} \\ x+1, & \text{If } x \text{ is odd.} \end{cases}$$

Use y as your output variable. Solution: See Figure 2.3.

2.4 Functions

Assume the universal set is non-negative integers. F is an n-argument function if f associates with each n-tuple $(x_1, x_2, ..., x_n)$ *at most one number.* If this number exists, it is called the *value of* f for the given arguments. If no number exists, then the function is undefined. An argument function f is a *total function* if f always computes a value for every n-tuple. Otherwise, f is a *partial function.*

Example: The addition function is *total.*

Example: The square root function is *partial.*

A program P *computes* a function F of n arguments with respect to a sequence of $n+1$ variables if for each n-tuple $x_1, x_2, ..., x_n$ when P is run with the first n variables of S as $x_1, ..., x_n$ input. Then,

1. If $f(x_1, ..., x_n)$ has a value then the program will halt in a finite amount of time and the $(n+1)^{st}$ variable of S has value $f(x_1, ..., x_n)$ at the halt.

2. If $f(x_1, ..., x_n)$ is undefined, then program P will never halt.

Skip Section 3.6.3 Verification in the textbook. Add a new command to the While language.

- DO x TIMES [program] — execute the program the number of times equal to the value of x when the command is first executed even if x changes.

Example: $x := 4$. DO x TIMES [INCR(x)]. The program part in the DO-TIMES loop gets executed 4 times.

A DO-TIMES program is a While language which *contains no While command.* It may contain DO-TIMES commands. This results in DO-TIMES programs that always halts. Every DO-TIMES can be written as a While command.

Homework: Chapter 3, page 82 # 1, 3 in the textbook.

2.4.1 Computable Functions

We wish to be able to describe the set of computable functions over the non-negative integers. We will study four types of formal definitions for functions:

1. Explicit definition.

2. Primitive recursion.

3. Mu recursion.

4. General equational definition.

Each of these is dependent on the concept of *functional expressions.*

1. Numeral — the same as in GOTO and WHILE.

2. Variable — one of x, y or z or one of these letters followed by a numeral subscript.

3. Function symbol — one of f, g or h or one of these followed by a numeral subscript. Can also be S for successor function. Also can be any symbol introduced by a function definition.

4. Functional expression of level 0 — a numeral or a variable.

5. Functional expression of level $i+1$ — At least one funct.expr is of level i; none are of level greater than i. For example, $f(4, x1, z5, 8)$ is level 1. Another example: $f(x, y, g(x), h(y, z))$ is level 2 because x, y is level 0 and $g(x)$ and $h(y, z)$ are level 1.

6. Equation — functional expression = function expressions.

An *explicit definition* of a function with n arguments is an equation with a function symbol followed by the argument variables on the left-hand side. The right side is a functional expression with no variables except those given as arguments and using only known function symbols.

Example: Assume that multiplication and addition are known function symbols. $f(x,y) = +(*(x,y,2) \approx x*y+2$.

Example: $g(z) = *(z, S(z)) \approx z*(z+1)$.

Example: $h(x,y,z) = +(+(*(3,x),y), *(2,z)) \approx (3x+y)+2*z$.

If functions g and h are known, then a *primitive recursion* definition of the n-argument function f from g and h is a pair of equations of the form

$$\begin{cases} f(x_1,x_2,...,x_{n-1},0) = g(x_1,x_2,...,x_{n-1}) \\ f(x_1,x_2,...,x_{n-1},S(x_n)) = h(x_1,x_2,...,x_n,f(x_1,x_2,...,x_n)) \end{cases}$$

Example: To define addition,

$$\begin{cases} +(x,0) = x \\ +(x,S(y)) = S(+(x,y)) \end{cases}$$

$+(3,2) = +(3,S(1)) = S(+(3,1))$. $+(3,1) = +(3,S(0)) = S(+(3,0)) = S(3) = 4 = S(4) = 5$.

Example: To define multiplication,

$$\begin{cases} *(x,0) = 0 \\ *(x,S(y)) = +(x,*(x,y)) \end{cases}$$

Example: To define factorial,

$$\begin{cases} f(0) = 1 \\ f(S(x)) = *(S(x),f(x)) \end{cases}$$

Example: To define exponentiation,

$$\begin{cases} \uparrow(x,0) = 1 \\ \uparrow(x,S(y)) = *(x,\uparrow(x,y)) \end{cases}$$

Notice that $0^0 = 1$ by this definition.

Example: To define the predecessor function,

$$\begin{cases} P(0) = 0 \\ P(S(x)) = x \end{cases}$$

Example: To define the floored subtraction,

$$\begin{cases} \dot{-}(x,0) = x \\ \dot{-}(x,S(y)) = P(\dot{-}(x,y)) \end{cases}$$

$\dot{-}(6,2) = \dot{-}(6,S(1)) = P(\dot{-}(6,1)) = \dot{-}(6,1) = (6,S(0)) = P(\dot{-}(6,0)) = P(6) = 5 = P(5) = 4$.

Example: To define the *signum function,*

$$\begin{cases} SG(0) = & 0 \\ SG(S(x) = & 1 \end{cases}$$

where

$$\left\{ SG(x) = \begin{array}{ll} 0 & \text{if } x = 0. \\ 1 & \text{if } x > 0. \end{array} \right.$$

Example: To define the *inverse of the signum function (SG),*

$$\left\{ \begin{array}{ll} ISG(0) = & 1 \\ ISG(S(x) = & 0 \end{array} \right.$$

Another way to state the inverse of the signum function is

$$\left\{ ISG(x) = \begin{array}{ll} 1 & \text{if } x = 0. \\ 0 & \text{if } x > 0. \end{array} \right.$$

Some more examples using explicit definitions follows.

Example: The *absolute difference* is defined as $ABD(x,y) = +(\dot{-}(x,y,\dot{-}(y,x))$ where if $x \leq y$ then $\dot{-}(x,y) = 0$ and $\dot{-}(y,x) = y - x$. If $x > y$, then $\dot{-}(x,y) = x - y$ and $\dot{-}(y,x) = 0$.

Example: The *maximum* function is defined as $\max(x,y) = +(x, \dot{-}(y,x))$ where if $x < y$, $+(x, y-x) = x + y - x = y$ and if $x \geq y$, $+(x, \dot{-}(y,x)) = +(x,0) = x$.

Example: The *minimum* function is defined as $\min(x,y) = \dot{-}(x, \dot{-}(x,y))$ where if $x < y$, $\dot{-}(x,0) = x$ and if $x \geq y$, $\dot{-}(x, x-y) = x - x + y = y$.

Example: The *greater-than* function is defined as

$$GT(x,y) = SG(\dot{-}(x,y)) = \left\{ \begin{array}{ll} 1 & \text{if } x > y. \\ 0 & \text{if } x \leq y. \end{array} \right.$$

Example: The *greater-than or equal-to* function is defined as

$$GE(x,y) = GT(S(x),y) = \left\{ \begin{array}{ll} 1 & \text{if } x \geq y. \\ 0 & \text{if } x < y. \end{array} \right.$$

Example: The *equal* function is defined as

$$EQ(x,y) = *(GE(x,y), GE(y,x)) = \left\{ \begin{array}{ll} 1 & \text{if } x = y. \\ 0 & \text{Otherwise.} \end{array} \right.$$

We can use these basic functions to define more complex functions.

Example: *Definition by cases.*

$$f(x) = \left\{ \begin{array}{ll} 3 & \text{if } x < 3. \\ 2x & \text{if } 3 \leq x \leq 6. \\ x - 2 & \text{if } x > 6. \end{array} \right.$$

The above function can be defined explicitly by $f(x) = 3 * GT(3,x) + 2x * GE(x,3) * GE(6,x) + \dot{-}(x,2) * GT(x,6)$.

Example: The *remainder* function. We wish to define the function $REM(x,y)$ equal to the remainder when x is divided by y. Recall if x is divided by y, then $x = y \cdot a + r$, $0 \leq r \leq y - 1$. Observation:

$$REM(x+1,y) = \left\{ \begin{array}{ll} 0 & \text{if } REM(x,y+1) = y. \\ REM(x,y)+1 & \text{Otherwise.} \end{array} \right.$$

Due to the way primitive recursive functions are given, we cannot define the function $REM(x, y)$ this way. So, we will define a new function f by primitive recursion such that:

$$REM(x,y) = f(x,y) = \begin{cases} f(y,0) = 0 \\ f(y,S(x)) = S(f(y,x))* \\ ISG(EQ(S(f(y,x)),y)) \end{cases}$$

This remainder function $REM(S(x), y) = [REM(x, y) + 1]$.

Example: The *quotient* function is explicitly defined as $QU(x, y)$ equal to the quotient where x is divided by y. Observation:

$$QU(x+1,y) = \begin{cases} Q(x,y) & \text{if } REM(x+1,y) \neq 0. \\ Q(x,y)+1 & \text{if } REM(x+1,y) = 0. \end{cases}$$

We will define g by primitive recursion such that

$$QU(x,y) = g(y,x) = \begin{cases} g(y,0) = 0 \\ g(y,S(x)) = g(y,x) + ISG(REM(S(x),y)) \end{cases}$$

Then, $QU(x + 1, y) = QU(x, y)+$ If $REM(x + 1, y) = 0$, then $ISG(REM...) = 1$.

Do the following problems on page 98 in the textbook. # 1, 2, 3, 4, 9, 12, 17. Test on Wednesday. It covers Chapter 1 algorithm requirements (understand steps), Labyrinth and Euclidean algorithms. Chapter 3. Know commands in languages, trace programs, write programs.

2.4.2 Homework and Answers

Problems on page 98 of the textbook.

Define the function described in each exercise by using primitive recursion or explicit definition or both, from the functions listed in Section 4.2.4 in the textbook. If possible, define the function entirely by means of explicit definition.

1. $MUL(x, y) = 1$ if x is an integral multiple of y. $MUL(x, y) = 0$ if not. Note that $MUL(0, y) = 1$ but $MUL(x, 0) = 0$ if $x \neq 0$. Solution:

$$MUL(x,y) = \begin{cases} 0 & \text{if } y = 0 \text{ and } x \neq 0. \\ 1 & \text{if } x = 0 \text{ and } y \neq 0. \\ SG((REM(y,x) & \end{cases}$$

2. $CON(x, y, z) = 1$ if $REM(x, z) = REM(y, z)$. $CON(x, y, z) = 0$ if $REM(x, z) \neq REM(y, z)$. Solution: $CON(x, y, z) = EQ(REM(x, z), REM(y, z))$.

3. $SD(x)$ is the sum of the positive integer divisors of x for $x \neq 0$. For example, $SD(1) = 1$. $SD(3) = 4$. $SD(6) = 12$. Solution:

$$SD(x) = \begin{cases} f(x,0) = 0 \\ f(x,y) = +(x, QU(x,S(u)) * ISG(REM(x,S(y)))) \end{cases}$$

4. $PR(x) = 1$ if x is prime. $PR(x) = 0$ otherwise. For example, $PR(0) = PR(1) = PR(4) = 0$. $PR(2) = PR(3) = PR(7) = 1$. Solution:

$$PR(x) = \begin{cases} 1 & \text{If } x \text{ is prime.} \\ 0 & \text{Otherwise.} \end{cases}$$

x is prime iff x has exactly two divisors. $D(x)$ counts the number of divisors of x. $PR(x) = EQ(D(x), 2)$.

9. $f(0) = 1$ for all x. $f(x+1) = \uparrow(2, f(x))$ if x is even. $f(x+1) = \uparrow(f(x), 2)$ if x is odd. Solution:

$$f(x+1) = \begin{cases} \uparrow(2, f(x)), & \text{If } x \text{ is even.} \\ \uparrow(f(x), 2), & \text{If } x \text{ is odd.} \end{cases}$$

$f(0) = 1$. $f(S(x)) = ISG(REM(x,2)) * \uparrow(2, f(x)) + SG(REM(x,2)) * \uparrow(f(x), 2)$.

12. Solution:

$$f(x,y,z) = \begin{cases} x+y, & \text{If } 50 \le x + y * z \le 100. \\ z, & \text{Otherwise.} \end{cases}$$

$f(x,y,z) = (x+y) * GE(x+y*z, 50) * GE(100, x+y*z) + z * GT(50, x+y*z) + z * GT(x+y*z, 100)$.

Assume $f, f_1, f_2, ...$ are given total functions of one argument whose mathematical nature you do not know. In each case, a one argument function h is described intuitively in terms of these. Define h by means of a primitive recursion or explicit definition.

17. $h(x) = \sum_{i=0}^{x} f(x)$. Solution:

$$h(x) = \sum_{i=0}^{x} f(i) = f(0) + f(1) + \cdots + f(x).$$

Note that $h(x+1) = f(0) + h(1) + \cdots + f(x) + f(x+1)$. Then,

$$h(x) = \begin{cases} h(0) = f(0) \\ h(S(x)) = h(x) + f(S(x)) \end{cases}$$

22. $h(x) = 1$ if both $f_1(x) = 1$ and $f_2(x) = 1$. $h(x) = 0$ otherwise. Solution: $h(x) = EQ(f_1(x), 1) * EQ(f_2(x), 1)$.

2.4.3 Primitive Recursion

Recall that we defined

1. Addition

$$\begin{cases} +(x, 0) = x \\ +(x, S(y)) = S(+(x, y)) \end{cases}$$

2. Multiplication

$$\begin{cases} *(x, 0) = 0 \\ *(x, S(y)) = +(x, *(x, y)) \end{cases}$$

3. Exponentiation

$$\begin{cases} \uparrow(x, 0) = 1 \\ \uparrow(x, S(y)) = *(x, \uparrow(x, y)) \end{cases}$$

Define:

- $\Phi_0(x, y) = S(y)$.
- $\Phi_1(x, y) = +(x, y)$.
- $\Phi_2(x, y) = *(x, y)$.
- $\Phi_3(x, y) = \uparrow (x, y)$.

Similarily, define $\Phi_4(x, 0) = 1$. $\Phi_4(x, S(y)) = \uparrow (x, \Phi_4(x, y))$. Notice that $\Phi_4(2, 0) = 1$ gives the next power. $\Phi_4(2, 1) = 2$. $\Phi_4(2, 2) = 4$. $\Phi_4(2, 3) = 2^4 = 16$. $\Phi_4(2, 4) = 2^{16} = 65536$. $\Phi_4(2, 5) = 2^{65536}$. In general, $\Phi_4(x, 0) = 1$. $\Phi_4(x, 1) = x^1 = x$. $\Phi_4(x, 2) = x^x$. $\Phi(x, 3) = x^{x^x}$. and so on. Likewise, define $\Phi_5 = (x, 0) = 1$. $\Phi_5(x, S(y)) = \Phi_4(x, \Phi_5(x, y))$. Verify that $\Phi_5(2, 4) = \Phi_4(2, 65536)$. Continuing in this manner, we can define an entire sequence of functions Φ_0, Φ_1, $\Phi_2, ...,$ Φ_i, $\Phi_{i+1}, ...$ such that

$$\Phi_{i+1}(x, 0) = 1$$
$$\Phi_{i+1}(x, S(y)) = \Phi_i(x, \Phi_{i+1}(x, y))$$

Notice that for each $x \geq 2$, $\Phi_{i+1}(x, y)$ increases faster with y than $\Phi_i(x, y)$. The *class of primitive recursive functions* consists of all functions which can be divided by explicit definition or primitive recursion. $\Phi_0, \Phi_1, \Phi_2, ...$ are in the class of primitive recursive functions. All functions in the class are computable. The *Ackerman function* (A) :

$$A(0, x, y) = S(y)$$
$$A(1, x, y) = +(x, y)$$
$$A(2, x, y) = *(x, y)$$
$$A(SSS(z), x, 0) = 1$$
$$A(SSS(z), x, S(y)) = A(SS(z), x, A(SSS(z), x, y))$$

In general, $A(i, x, y) = \Phi_i(x, y)$. A is computable, but A is not in the class of primitive recursive functions (not primitive recursion and not explicit either). The trivial cases of S, $+$, $*$, and $\uparrow$ are not the same as the Ackerman function. If we define $h(x) = A(x, x, x)$ then h increases faster than any one-argument primitive-recursion function.
We wish to formally show how to compute the value of a function. We will begin with a set of equations which define the function and generate a sequence of equations which ends with the evaluation. Some definitions and notation:

- *An evaluation* — $*(3, 5) = 15$.
- *Rule of uniform substitution* — Given $*(x, S(y)) = +(x, *(x, y)) \Rightarrow *(3, S(y)) = +(3, *(3, y))$.
- *Rule of evaluation replacement* — Given $*(4, 0 = 0$, $*(4, 1) = +(4, *(4, 0)) \Rightarrow *(4, 1) = +(4, 0)$.

The fourth means to define a function: An n argument function, Q, is *equationally defined* by a set of equations, Φ, if for every n-tuple $(i_1, i_2, ..., i_n)$, no two distinct evaluations for $Q(i_1, i_2, ..., i_n)$ are derived from Φ. All explicit, primitive recursion, and mu recursion definitions can be converted to equational definitions.

2.4.4 Mu Recursion

Add μ and [] to our syntax for defining functions. A *mu expression* has the form $(\mu V)[E = 0]$ where V equals a variable and E equals an expression. The minimum value of V such that $E = 0$. A *mu recursion definition* of an f with n arguments has the form $f(x_1, x_2, ..., x_n) = (\mu V)[$ functional expression $= 0]$ where the functional expression has only $x_1, x_2, ..., x_n, V$. We will assume that the functional expression contains no mu expressions and that it contains only function symbols for total functions.

Example: $f(x, y) = (\mu z)[ISG(EQ(y * z, x)) = 0]$ i.e. $f(x, y)$ equals to the smallest value of z such that $y * z = x$. $f(8, 4) = (\mu z)[ISG(EQ(4 * z, 8)) = 0] = 2$. $f(7, 4)$ has no value.

$f(x,y) = (\mu z)[\dot{-}(x,z) = 0]$. $f(3,7) = (\mu z)[\dot{-}(3,2) = 0] = 3$, $3 - 2 = 0$.

Define $f(x,y)$ to be the least common multiple of x and y. If either $x = 0$ or $y = 0$, then let $f(x,y) = 0$. If $z = LCM(x,y)$, then z is the smallest number such that z is divisible by x and y. $f(x,y) = (\mu z)[x * y * (ISG(z) + REM((z,x) + REM(z,y)) = 0]$.

1. If x or y equal to zero, then z is zero. Consider $f(x,y) = 0$.
2. If neither x nor y equal to zero, consider $f(3,6) = (\mu z)[3 * 6 * (ISG(z) + REM(z,3) + REM(z,6)) = 0] = 6$.

f can be defined in two steps as follows:

1. Explicit — $g(x,y,z) = x * y * (ISG(z) + REM(z,x) + REM(z,y))$.
2. Mu Recursion — $f(x,y) = (\mu z)[g(x,y,z) = 0]$.

Example: Another definition for the quotient. Recall if x is divided by y, then $x = y \cdot a + r$. $\Rightarrow x \geq y \cdot a$ and $\Rightarrow y \cdot a \leq x$. So, define $QU(x,y)$ equal to the *largest* non-negative integer, w, such that $w \cdot y = x =$ the smallest z such that $z \cdot y > x - 1$. To illustrate, $QU(7,3) =$ largest w where $w \cdot 3 \leq 7 \Rightarrow w = 2$. $QU(7,3) =$ smallest z where $z \cdot > 7 - 1 \Rightarrow z = g(x,y) = (\mu z)[y * ISG(GT(z * y, x)) = 0]$. $QU(x,y) = P(g(x,y))$. $QU(x,0) = (\mu z)[0 * \cdots = 0] = 0$. $QU(x,0) = P(0) = 0$.

Since mu recursive definitions can lead to partial functions, we see that there is a relationship between mu recursion functions and the halting problem.

Example: $f(x) = (\mu z)[\uparrow(z,2) = x]$ is the partial square root function. $z = 5$ is an example.

Example: $g(x,y) = (\mu z)[ISG(z) + REM(z,x) + REM(z,y) = 0]$ is the partial positive least common multiple function. g is undefined when $x = 0$ or $y = 0$. Programs for defined functions include:

- If f is defined explicitly in terms of other functions for which the While-language programs exist, then it is possible to write a While-language program with *no new loops* which computes f. See Section 4.5.1 in the textbook.
- The previous result applies for the Goto-language, also.
- If f is defined by primitive recursion in terms of other functions for which the While-language programs exist, then it is possible to construct a DO-TIMES program which computes f. See Section 4.5.2 in the textbook.
- If f is defined by a sequence of explicit definitions and primitive recursions, then f is computable by the DO-TIMES program.
- If f is defined by mu recursion in terms of total functions which has a While-language program, then f can be computed by a While-language program. See Section 4.5.3 in the textbook. The program for f may not always halt.

Some additional results include:

- Any function which is computed by a DO-TIMES program is in the *class of primitive recursion functions.* This means it can be defined from the successor function by a sequence of explicit definitions and primitive recursions.
- Any function, partial or total, which can be computed by a While-language program can be defined by *repeated applications of explicit definitions, primitive recursions, and mu recursion.* This is the class of *mu-recursion functions.*

- A function is *mu-recursive* if it can be defined in a sequence of steps from the successor function by explicit definition, primitive recursion, and mu recursion.
- A function is *equationally definable* if it can be equationally defined in the formalism of functional expressions.

All classes of functions are equal. This is the class of computable functions.

Homework: problems on page 119, #1, 3, 5, 7.

2.4.5 Homework and Answers

Problems from page 119 in the textbook.

1. Assume as given, the function PR where $PR(x) = 1$ if x is prime; and $PR(x) = 0$ if x is not prime. (a) Define f from PR by mu recursion where $f(x)$ is the smallest prime number greater than x. (b) Define g by mu recursion, possibly with the help of explicit definition, where $g(x)$ is the greatest prime number less than x. Note that g is a partial function since $g(0), g(1)$ and $g(2)$ have no values. (c) By means of primitive recursion from f, define the one-argument function $PRIME$ where $PRIME(x)$ = the x^{th} prime in order of magnitude counting 2 as the zero-th prime. Thus $PRIME(0) = 2$. $PRIME(1) = 3$.

a. Solution: $f(x) =$ smallest prime $> x$. $f(x) = (\mu z)[ISG(PR(z) * GT(z, x)) = 0]$.

b. Solution: $g(x) =$ greatest prime $< x$. Find $z = \dot{-}(x, w)$ such that z is minimized. Note that $w = \dot{-}(x, z)$.

$$\begin{cases} h(x) = (\mu z)[ISG(PR(\dot{-}(x, z))) + ISG(z) = 0] \\ g(x) = \dot{-}(x, h(x)) \end{cases}$$

c. Solution: Prime(0) = 2. Prime(1) = 3. Prime(2) = 5. Prime(3) = 7. $f(x) =$ smallest prime $> x$. By primitive recursion, Prime(0) = 2; Prime($S(x)$) = f(Prime(x)).

3. Define each of the two functions by mu recursion, possibly with the help of explicit definition. (a) $g(x) = 0$ if x is a perfect square. Otherwise $g(x)$ has no value. (b) $h(x) = 0$ if x is not a perfect square. Otherwise $h(x)$ has no value.

a. Solution:

$$g(x) = \begin{cases} 0 & \text{If } x \text{ is a perfect square.} \\ \text{No value} & \text{Otherwise.} \end{cases}$$

$$\begin{cases} h(x) = (\mu z)[ISG(EQ(\uparrow(z, 2), x)) = 0] \\ g(x) = *(0, h(x)) \end{cases}$$

If x is not a perfect square, then $h(x)$ has no value.

b. Solution:

$$h(x) = \begin{cases} 0 & \text{If } x \text{ is not a perfect square.} \\ \text{No value} & \text{Otherwise.} \end{cases}$$

$z^2 < x < (z+1)^2$. $h_1(x) = (\mu z)[ISG(GT(x, z^2) * GT((z+1)^2, x)) = 0]$. $h(x) = ISG(h_1(x))$ or $z^2 > x$ and $h_1(x) = (\mu z)[ISG(GT(z^2, x)) = 0]$. L. J. Randall's comment: One idea is to look at $(z-1)^2$. Case 1: $(z-1)^2 = x$. Case 2: $(z-1)^2 \neq x$. $h(x) = (\mu z)[EQ(P(h_1(x))^2, x) = 0]$ for the case $(z-1)^2 \neq x$.

In each exercise, define the two functions described using mu recursion, possibly with the help of explicit definition, but without using primitive recursion. The function you define in part (a) of each exercise must not have a value precisely where the specification calls for it not to have a value. The function you define in part (b) must be a total function.

5a.

$$f(x,y) = \begin{cases} x+2y & \text{If } x \neq y. \\ \text{Undefined} & \text{Otherwise.} \end{cases}$$

Solution: $f(x,y) = (\mu z)[ISG(EQ(z, x+2y)) + EQ(x,y) = 0]$.

5b.

$$g(x,y) = \begin{cases} x+2y & \text{If } x \neq y. \\ 0 & \text{If } x = y. \end{cases}$$

Solution: $g_1(x,y) = (\mu z)[ISG(EQ(z, x+2y)) = 0]$. $g(x,y) = ISG(EQ(x,y)) * g_1(x,y)$.

7a.

$$f(x,y) = \begin{cases} \text{Largest } w \leq x \text{ and } h(w) = y \\ \text{No value if no } w \text{ exists.} \end{cases}$$

Solution: The smallest z will produce the largest w. $z = \dot{-}(x,w)$ or $w = \dot{-}(x,z)$. $f_1(x,y) = (\mu z)[ISG(EQ(h(\dot{-}(x,z)),y))+$ $ISG(GE(x,z)) = 0]$. $f(x,y) = \dot{-}(x, f_1(x,y))$.

7b. Solution: $f_2(x,y) = (\mu z)[ISG(EQ(h(\dot{-}(x,y)),y)) * ISG(EQ(x,z)) = 0]$. $f(x,y) = \dot{-}(x, f_2(x,y))$.

2.4.6 Formal Computations Summary

A *formal computation* is a derivation of an evaluation from a given set of evaluations.

Example: The following shows a formal computation of $\dot{-}(3,1)$ for Φ.

$$\Phi = \begin{cases} \dot{-}(x,0) = x \\ \dot{-}(x,S(y)) = P(\dot{-}(x,y)) \\ P(0) = 0 \\ P(S(x)) = x \end{cases}$$

- For the class of primitive-recursive functions, these are all functions which can be defined by a sequence of explicit definitions and primitive recursions.
- Total functions — given the definition of a function in this class, we can write an algorithm to compute the function. Every function in this class is computable by a DO-TIMES program. These programs always halt.
- Not all primitive recursive functions are practically computable.
- All computable functions can be defined by a mu-recursive and an explicit definition. This is a major result.

The following four definitions are equivalent:

1. A function is *Turing computable* if it possible to construct a Turing machine that computes it.
2. A function is *program computable* if it is possible to write a program (Goto, While) that computes it.
3. A function is *mu-recursive* if it can be defined in a sequence of steps from the successor function by explicit definition, primitive recursion, and mu recursion.
4. A function is *equationally definable* if it can be equationally defined in the formalism of functional expressions.

All classes of functions are equal. This is the class of computable functions.
Omit Section 4.7 in the textbook.

Skip Chapters 5 and 6 in the textbook.

2.5 Context Free Grammars

A *grammar* is a formal description of the syntax of a formal language. A *context free grammar* consists of:

1. A set of characters called the *terminal alphabet.*
2. A set of characters called the *non-terminal alphabet,* disjoint from the set in (1).
3. The *start symbol* — a character from the non-terminal alphabet.
4. A set of *productions* of the form: non-terminal → character string, where the character string may consist of both terminal and non-terminal characters.

Example: A simplified version of the language of functional expressions.

Assume that there are:

1. Two functional symbols: S and $+$.
2. Three variables x, y, and z.
3. Binary numbers only.

The terminal alphabet is: $S, +, x, y, z, 0, 1,$ (,), comma, $<, >$. We can generate only binary numeral N with the following productions:

$N \to 0$
$N \to 1$
$N \to 1R$
$R \to 0R$
$R \to 1R$
$R \to 0$
$R \to 1$

To use a production, replace the non-terminal on the left of the arrow with the string on the right. A *derivation* to show that 1100 is a numeral is as follow:

N start symbol
$1R$
$11R$
$110R$
1100

0110 is not possible using the above productions. A derivation to show that 1100 is a numeral is as follow:

N start symbol
$1A$
$11A$
$110A$
1100

We can generate any variable V with the following productions:

$V \to x$
$V \to y$
$V \to z$

The functional expression E can be generated by:

$$
\begin{aligned}
&E \to N\\
&E \to V\\
&E \to +(E, E)\\
&E \to S(E)
\end{aligned}
$$

An equation Q needs only one production: $Q \to E = E$. A derivation to show that $+(+S(x)), 11), S(0)$ is a functional expression is as follow:

$$
\begin{aligned}
&E \text{ Start symbol}\\
&+(E, E)\\
&+(+(E, E), E)\\
&+(+(S(E), E), E)\\
&+(+(S(V), E), E)\\
&+(+(S(x), E), E)\\
&+(+(S(x), N), E)\\
&+(+(S(x), 1A), E)\\
&+(+(S(x), 11), E)\\
&+(+(S(x), 11), S(E))\\
&+(+(S(x), 11), ...
\end{aligned}
$$

This is in the textbook.

In a grammar, one type of production is chosen as being the most important. In our example, we will choose the set of Equations Q. Q will be the *start symbol* of the grammar and henceforth all derivations in the derivation will start with Q. The *language* of a context-free grammar is the set of strings over the terminal alphabet that are derivable from the start symbol. If G is a context-free grammar, then we denote the language of G by $L(G)$. The grammar defines the language. Summary:

1. Terminal alphabet $S, +, x, y, z, 0, 1,$ (,), comma.
2. Non-terminal alphabet N, A, V, E, Q.
3. Start symbol Q.
4. Productions:

$$
\begin{aligned}
&Q \to E = E\\
&N \to 0|1|1A\\
&A \to 0A|1A|0|1\\
&V \to x|y|z\\
&E \to +(E, E)|S(E)|N|V
\end{aligned}
$$

Page 197 in the textbook gives the full formalism of functional expressions. The more grammars, the more productions. $\{1-3\}$ are numerals. $\{4\}$ are variables. $\{5-12\}$ are functional expressions. $\{13\}$ are a sequence of functional expressions. $\{14\}$ is equations. Page 198 in the textbook gives a context free grammar for the GOTO language. $\{1-3\}$ is names. $\{4-5\}$ is unlabeled commands. $\{6\}$ is labeled commands. $\{7\}$ is programs. $\{8-10\}$ is numerals.

$$
\begin{aligned}
&\delta \to ...\\
&\gamma \to ...\\
&\alpha \to ...
\end{aligned}
$$

are the same as numerals in the previous expressions.

Example: A context-free grammar, G-IN, for propositional calculus that uses parenthesis. Assumptions:

1. Only operators are $\delta, \vee$, and $\approx$.
2. Only variables are $p, q, r, p', q', r', p'', q'', r'', \ldots$.
3. The terminals are $\delta, \vee, \approx, p, q, r, \prime, (,)$.
4. The non-terminals are s, A.
5. The start symbol is s.
6. Productions — see page 199 in the textbook. $s \to$ and $A \to$.

Example: $p \vee \approx q$ is not possible. But $(p) \vee (\approx (q))$ is possible.

s
$(s) \vee (s)$
$(A) \vee (A)$
$(p) \vee (q)$

Example: A grammar, G-PRE, for parenthesis free propositional calculus. See page 202, bottom in the textbook. $p \vee q \approx \vee pq$.

Example: A grammar, G-Suf, for parenthesis free propositional calculus in suffix form. See page 203 in the textbook.

Example: Describe the language of the grammar. Given: $S \to cS|bD|c$. $D \to cD|bS|b$. Start symbol is S. Terminals c, b. Generate strings:

S	S
c	cS
	ccS
	$cccS$

$\vdots$
$ccc\cdots c$

S	S	S
bD	bD	bb
	$bccD$	$bccD$
	$bcccb$	$bcccD$
	$bcccb$	$bcccbS$
		$bcccbc$

All strings in this language have an even number of $b's$.

Example: A grammar for the set of palindromes over the alphabet $\{b, c\}$. $S \to bSb|cSc|bb|cc|b|c$. Derive $bbcbcbcbb$.

S
bSb
$bbSbb$
$bbcScbb$
$bbcbSbcbb$
$bbcbcbcbb$

Example: A grammar for $\{b^m c^n d^n e^m | m, n \geq 1\}$. $S \rightarrow bSe|bJe$. $J \rightarrow cJd|cd$. Note that $b^3 = bbb$. Derive $b^3c^2d^2e^3$.

S
bSe
$bbSee$
$bbbJeee$
$bbbcJdeee$
$bbbccddeee$

Example: A grammar for $\{b^m c^n d^n e^m f^p (gh^*)^p | m \geq 2, n \geq 0, p \geq 1\}$.

$S \rightarrow JK$
$J \rightarrow bJe|bbee|bbLee$
$L \rightarrow cLd|cd$
$K \rightarrow fKQ|fQ$
$Q \rightarrow Qh|g$

Note that h^* represents $h^n \geq 0$. Derive $b^3c^2d^2e^3f^4(gh^*)^4$.

S
JK
$bJeK$
$bbbLeeeK$
$bbbcLdeeeK$
$bbbccddeeeK$
$bbbccddeeeKfKQ$
$bbbccddeeeKffKQQ$
$bbbccddeeeKfffKQQQ$
$bbbccddeeeKffffQQQQ$
$bbbccddeeeKffffQhQQQ$
$bbbccddeeeKffffghQQQ$

2.5.1 Exam 2 and Answers

All functions on this exam are defined over the non-negative integers.

1. Define function g by explicit definition where

$$g(x, y) = \begin{cases} x + y, & \text{If } x \text{ is even.} \\ y^x, & \text{If } x \text{ is odd.} \end{cases}$$

   Solution: $ISG(REM(x, 2)) * (x + y) + REM(x, 2) * (\uparrow (y, x))$.

2. Define function h by primitive recursion where $h(0) = 3$ and $h(x + 1) = 2 * h(x)$ if $0 < x < 10$, and $h(x + 1) = 3 * h(x)$ if $x \geq 10$. Solution:

$$h(x + 1) = \begin{cases} h(0) = 3 \\ h(S(x)) = GT(x, 0) * GT(10, x) * 2 * h(x) + GE(x, 10) * 3 * h(x) \end{cases}$$

3. Assume that f_1 and f_2 are known total functions. Define h such that:

$$h(x) = \begin{cases} 1, & \text{If } f_1(x) = 1 \text{ or } f_2(x) = 1 \text{ or both.} \\ 0, & \text{Otherwise.} \end{cases}$$

4. Give a mu-recursive definition of function f such that $f(x, y)$ is the smallest $z \leq x$ such that $h(z) = y$. $f(x, y)$ has no value if there is no such z. Assume that h is some known total function of one argument. Solution: $f(x, y) = (\mu z)[ISG(EQ(h(z), y)) + ISG(GE((x, z)) = 0]$.

5. Consider the following definition of function g. Find $g(15)$.

$$f(x) = (\mu z)[ISG(GT(x, *(2, \dot{-}(x, z))))) = 0]$$
$$g(x) = \dot{-}(x, f(x))$$

Solution:

$g(15) = \dot{-}(15, f(15) = \dot{-}(15, 8) = 7$	
$f(15) = (\mu z)[ISG(GT(15, *(2, \dot{-}(15, z)))) = 0]$	
$z = 1$	$ISG(GT(15, 2 * 14))$
	$GT(15, 28)$
$z = 2$	$ISG(GT(15, 2 * 13))$
	$GT(15, 26)$
$z = 3$	$ISG(GT(15, 2 * 12))$
	$GT(15, 24)$
$z = 4$	$ISG(GT(15, 2 * 11))$
	$GT(15, 22)$
$z = 5$	$ISG(GT(15, 2 * 10))$
	$GT(15, 20)$
$z = 6$	$ISG(GT(15, 2 * 9))$
	$GT(15, 18)$
$z = 7$	$ISG(GT(15, 2 * 8))$
	$GT(15, 16)$
$z = 8$	$ISG(GT(15, 2 * 7))$
	$GT(15, 14)$
	$ISG(1) = 0$

6. Define the class of primitive recursive functions. Given an argument to show that this class contains infinitely many functions.

7. Describe (by giving a formula) the language of the following grammar.

$$S \to bSc|H$$
$$H \to aHd|add$$

8. Give a context-free grammar for the following set of strings. $\{x^n b^{2n-1} c | n \geq 1\}$.

9. Give a context-free grammar which uses λ productions for $\{(d^*c)^n (ab^*)^{2n} | n \geq 0\}$.

2.5.2 Lambda Productions

Let λ denote the null string. If we concentrate λ with any s, we obtain s. $\lambda s = s\lambda = s$. Consider a context free grammar for $\{b^m c^n | m \geq 0, n \geq 1\}$. To generate $b^m, m \geq 0$ we can use $B \to \lambda|bB$. To generate $c^n, n \geq 1$ we use $H \to c|cH$. Now to get $b^m c^n$, we use $S \to BH$. This grammar can be written without a lambda production.

$$S \to c|bS|bH|cH$$
$$H \to c|cH$$

Example: Write a context free grammar for $\{b^m c^m h d^n e^n h f^p g^p | m, n, p \geq 0\}$.

$$S \to BhDhF$$
$$B \to bBc|\lambda$$
$$D \to dDe|\lambda$$
$$F \to fFg|\lambda$$

This grammar can be written without lambda productions.

It is always possible to convert a context free grammar with λ productions into a context free grammar with out lambda productions. If λ is in the first language, it will not be in the second language. There are three steps to convert G_0 to a grammar without lambda productions.

Step 1: Identify all non-terminals which can yield λ, either directly or indirectly. For example,

$$
\begin{aligned}
&S \rightarrow eSe\\
&S \rightarrow CD\\
&C \rightarrow fCg\\
&C \rightarrow \lambda\\
&D \rightarrow \lambda\\
&B \rightarrow hB\\
&B \rightarrow f
\end{aligned}
$$

Step 2: Construct G_1 from G_0 as follows:

1. Identify each production of G_0 which has at least one λ-yielding non-terminal on the right side.
2. Suppose the production identified in (1) has the form $B \rightarrow \cdots G_1 \cdots G_2 \cdots G_p \cdots$ where $G_1, G_2, ..., G_p$ are λ-yielding productions.
3. Add to the list of productions all those that can be formed by deleting a *non-empty subset* of $\{G_0, G_1, ..., G_p\}$ from the right side.

Step 3: Construct G_0 from G_1 by deleting. For example, for G_1,

$$
\begin{aligned}
&S \rightarrow eSe|ee\\
&S \rightarrow CD|D|C|\lambda\\
&C \rightarrow fCg|fg\\
&C \rightarrow \lambda
\end{aligned}
$$

gets converted into:

$$
\begin{aligned}
&D \rightarrow BDh|Bh\\
&D \rightarrow \lambda\\
&B \rightarrow hB\\
&B \rightarrow f
\end{aligned}
$$

Another example, G_2 :

$$
\begin{aligned}
&S \rightarrow eSe|ee\\
&S \rightarrow CD|D|C\\
&C \rightarrow fCg|fg
\end{aligned}
$$

gets converted into:

$$
\begin{aligned}
&D \rightarrow BDh|Bh\\
&B \rightarrow hB\\
&B \rightarrow f
\end{aligned}
$$

Do problems 1, 3, 5, 6, 7, 11 on page 212 in the text book.

2.5.3 Homework and Answers

Page 212 in the textbook.

Give a formula for the language of each of the following grammars.

1.

$$S \to bbSc|H$$
$$H \to cHdd|cd$$

Solution: $\{b^{2n}c^m d^{2m-1}e^n | n \geq 0, m \geq 1\}$.

3.

$$S \to HSKK|HK$$
$$H \to bH|c$$
$$K \to Kc|d$$

Solution: $\{(b^*c)^n(de^*)^{2n-1} | n \geq 1\}$.

$$S \to (H)^n(K)^{2n-1}$$
$$H \to b^*c$$
$$K \to de^*$$

5. $S \to bSc|bScc|bSccc|bc$. Solution: $\{b^n c^m | n \geq 1, n \leq m \leq 3n-2\}$.

S
$bSccc$
$bSccccc$
$bbbcccccc$

In each exercise, give a context-free grammar for the set of strings described. Exclude the null string from consideration.

6. $\{b^{m+n}c^m d^n | m \geq 0, n \geq 1\}$. Solution:

$$S \to bSd|bTd|bd$$
$$T \to bTc|bc$$

7. $\{b^{m+n}c^m d^n | m \geq 1, n \geq 0\}$. Solution:

$$S \to bSd|T$$
$$T \to bTc|bc$$

11. $\{(d^*c)^m(c^*d)^m | m \geq 2\}$. Solution:

$$S \to HSK|HHKK$$
$$H \to dH|c$$
$$K \to cK|d$$

2.5.4 Homework and Answers

Page 228 in the text book.

1. Construct G_1 and G_2 where G_0 is

$$\begin{aligned}&S \to bEf\\ &E \to bEc|GGc\\ &G \to b|KL\\ &K \to cKd|\lambda\\ &L \to dLe|\lambda\end{aligned}$$

Solution: G, K, L can produce λ. G_0 is in the text book. G_1 is:

$$\begin{aligned}&S \to bEf\\ &E \to bEc|GGc|Gc|c\\ &G \to b|KL|L|K|\lambda\\ &K \to cKd|cd|\lambda\\ &L \to dLe|de|\lambda\end{aligned}$$

G_2 is

$$\begin{aligned}&S \to bEf\\ &E \to bEc|GGc|Gc|c\\ &G \to b|KL|L|K\\ &K \to cKd|cd\\ &L \to dLe|de\end{aligned}$$

Note that $\lambda \neq L(G_0)$ and that $\lambda \neq L(G_2)$.

2.5.5 Parsing

To *parse* a string means to determine the structural meaning of the string. For example, strings of a high-level programming language must be parsed to be translated into machine code. We wish to study ambiguities in formal languages. There are two types of ambiguity:

1. *Lexical ambiguity* — here a symbol or expression has more than one meaning.

2. *Structural ambiguity* — a string can be parsed into more than one way, giving it different meanings.

Formal languages should be free of structural ambiguities. If a context-free grammar is used to describe the syntax of a language, then a derivation tree can be used to parse a string of the same language. If a string has more than one derivation tree, then it has more than one structural meaning and is structurally ambiguous. A *context-free* grammar is *ambiguous* if there is a string in the language of the grammar that has at least two *non-isomorphic* derivation trees.

Example: $S \to bS|Sb|c$ is an ambiguous grammar. See Figure 2.4. Change to

$$\begin{aligned}&S \to bS|A\\ &A \to Ab|c\end{aligned}$$

which is isomorphic.

How can we change an ambiguous grammar into an unambiguous one? One possible solution is to modify the language. This might be done by adding parenthesis or by changing to prefix notation. Suppose we do not want to modify the language to remove ambiguities. Then we must try to change the grammar for the language.

Example: $S \to bS|cS|bbS|\lambda$ is ambiguous. See Figure 2.5. The solution is $S \to bS|cS|\lambda$.

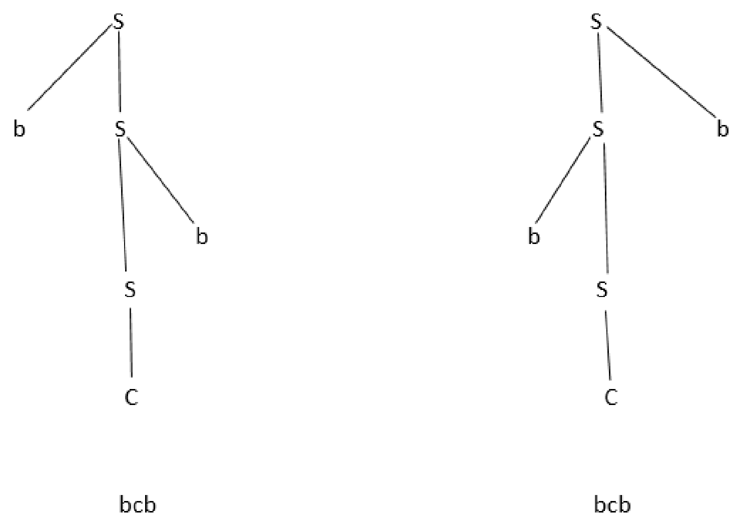


Figure 2.4: This figure shows the ambiguous grammar example

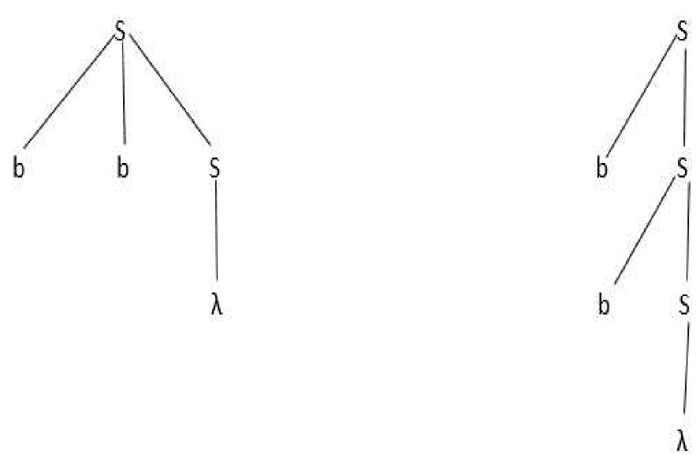


Figure 2.5: This figure shows the ambiguous grammar example

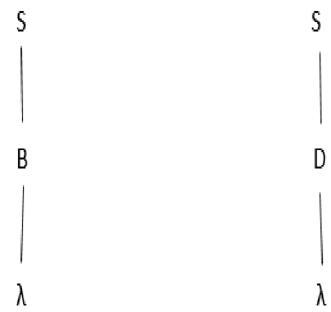


Figure 2.6: This figure shows the ambiguous grammar example

Example: The following is ambiguous

$S \to B|D$
$B \to bBc|\lambda$
$D \to dDe|\lambda$

See Figure 2.6. The solution is

$S \to B|D|\lambda$
$B \to bBc|bc$
$D \to dDe|de$

Result: Some ambiguities in a context-free grammar may not have an unambiguous equivalent. The corresponding language is said to be *inherently ambiguous.* Some more results:

1. There is no decision procedure to tell whether or not a grammar is ambiguous.
2. There is no decision procedure to tell whether or not a grammar is inherently ambiguous.
3. There is no algorithm for converting an ambiguous context free grammar into an unambiguous one.

For homework, do problems 7, 9, 11, 13, 15 on page 247 in the textbook.

2.6 Regular Languages and Finite Automata

A *regular grammar* is a context-free grammar in which every production has as its right side either

1. A terminal followed by a non-terminal.
2. A single terminal.
3. λ.

A language is regular if there is a regular grammar for it.

Example: G :

$S \to cS|bD|\lambda$
$D \to cD|bS$

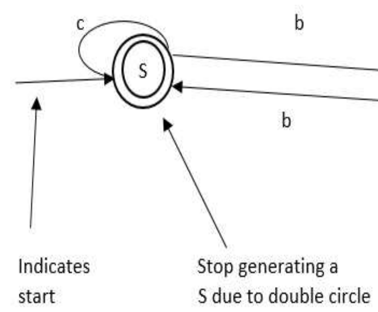


Figure 2.7: This figure shows a directed graph

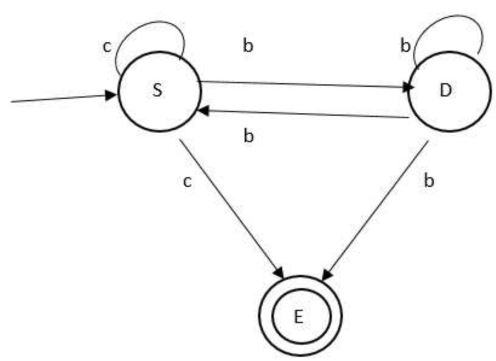


Figure 2.8: This figure shows a one-to-one correspondence

Regular grammars generate strings left to right. A *reverse regular grammar* is a context-free grammar which generates strings right to left.

Example: G' :

$$S \to Sc|Db|\lambda$$
$$D \to Dc|Sb$$

Notice that $L(G') = L(G)$.

Every regular grammar can be represented by a directed graph in which nodes correspond to non-terminals and arcs correspond to productions. See Figure 2.7.

Example: G_1 :

$$S \to cS|bD|c$$
$$D \to cD|bS|b$$

See Figure 2.8. There is a one-to-one correspondence between the walks in the graph and the strings in the grammar.

A *transition graph* is a directed graph whose arcs are labelled by characters from an alphabet. One node is the *start node.* One or more nodes are *accepting nodes* indicated by the double circles. The *language* of a

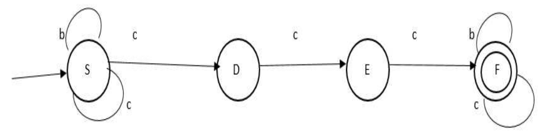


Figure 2.9: This figure shows the transition graph for the regular grammar

transition graph is the set of all strings generated by all walks from the start node to the accepting nodes. Every regular grammar has an equivalent transition graph and every transition graph has an equivalent regular grammar.

Example: Consider the regular grammar:

$$S \to bS|cS|cD$$
$$D \to cE$$
$$E \to cF$$
$$F \to bF|cF|\lambda$$

See Figure 2.9 for the transition graph.

We wish to consider a *finite automata* which is a language recognition device. A *finite automata* has a finite amount of memory. It has as input a string written on an input tape. Its goal is to determine whether the string is "acceptable." A *deterministic finite automata* consists of:

1. The machine alphabet G. These are the characters which it can read.
2. A finite set of states, K.
3. One element of K called the start state.
4. A subset of K called the accepting states.
5. A transition function $t : K \times G \to K$ where $\times$ is the Cartesian product and t maps T : (state, char) $\to$ state.

The automata begins in the start state. It reads the leftmost non-blank square on the input tape and proceeds according to the transition function. Then it goes one square to the right on the input tape. If the automata halts in an accepting state, the string is accepted; otherwise it is rejected. The language of the automata is the set of all strings over the machine alphabet that it accepts.

Example: The following defines an automata:

1. Machine alphabet $\{c, d\}$.
2. States S, Q, R.
3. Start state S.
4. Accepting state Q.
5. Transition function t :

$$t(S, L) = t(Q, c) = S$$
$$t(S, c) = Q$$
$$t(Q, b) = t(R, b) = t(R, c) = R$$

2.6.1 Regular Expressions

We will define a general regular expression. Each general regular expression denotes a set of strings. We will see that every general regular expression corresponds to a regular language. Let α and β be *sets* of strings. The *concatenation* of $\alpha\beta$ is given by $\alpha\beta = \{xy | x \in \alpha, y \in \beta\}$.

Example: $\alpha = \{b, bc, bcb\}$. $\beta = \{c, bb\}$. $\alpha\beta = \{bc, bbb, bcc, bcbb, bcbc, bcbbb\}$.

In general, $\alpha\beta \neq \beta\alpha$, is not commutative. If $\alpha = \{\lambda\}$, then $\alpha\beta = \beta$. If $\alpha = \emptyset$, then $\alpha\beta = \emptyset$. If α is a set of strings, then

1. $\alpha^0 = \{\lambda\}$.
2. $\alpha^{n+1} = \alpha\alpha^n$.

Example: $\alpha = \{a, b\}$. $\alpha^0 = \{\lambda\}$. $\alpha^1 = \alpha\alpha^0 = \{a, b\}$. $\alpha^2 = \alpha\alpha^1 = \{aa, ab, ba, bb\}$. $\alpha^3 = \alpha\alpha^2 = \{aaa, aab, aba, abb, baa, bab, bba, bbb\}$.

Let α be a set of strings. The *star closure* of α is denoted by α^* and is given by $\alpha^* = \bigcup_{n=0}^{\infty} \alpha^n = \alpha^0 \cup \alpha^1 \cup \alpha^2 \cdots$. $\alpha^* = G^*$ equals to all strings over G.

Example: $\alpha = \{b, bc\}$. $\alpha^* = \{\lambda, b, bc, bb, bbc, bc, bb, bbc, bcb, bcbc, ...\}$.

Definition: Let G be a string alphabet. Then,

1. $\emptyset$, $\{\lambda\}$, and $\{w\}_{w \in G}$ are general regular expressions.
2. If α and β are general regular expressions, then so are:
   (a) $(\alpha) \cup (\beta)$.
   (b) $(\alpha) \cap (\beta)$.
   (c) $(\alpha) - (\beta)$.
   (d) $(\alpha)^n$.
   (e) $(\alpha)^*$.

Notation: we will write b instead of $\{b\}$, c^* instead of $\{c\}^*$ and bc^*d instead of $\{b\}\{c\}^*\{d\}$. The precedence of operations is in this order:

1. Star, exponents.
2. Concatenation
3. Union, intersection, and difference.

Rule: parenthesis may be omitted only when operators are in different classes. For example, $\alpha^*\beta \cap \gamma$ means $(\alpha)^*(\beta) \cap \gamma$.

Example: $b^* = \{\lambda, b, bb, bbb, ...\}$ is the set of all strings over $\{b\}$.

Example: $(b \cup c)^* = \{\lambda, b, c, bb, bc, cb, cc, ...\}$

Example: $(a \cup b)^*a = \{a, b\}^*\{a\}$ is the set of all strings over $\{a, b\}$ which end in "a."

Example: $(b \cup c)^*bbb(b \cup c)^*$ is the set of all strings over $\{b, c\}$ having "bbb" as a substring.

Example: $(b \cup c)^* bbb(b \cup c)^* \cap (b \cup c)^* ccc(b \cup c)^*$ is the set of all strings over $\{b, c\}$ containing a substring "bbb" and a substring "ccc."

Example: a^*b^* is the set of all strings in which all $a's$ come before $b's$.

Example: $(aa)^* = \{\lambda, aa, aaaa, aaaaaa, ...\}$.

Example: $(a \cup c)b^* = \{a, c, abbb, ..., cbbb, ...\}$.

Example: Give a regular expression for the set of all strings of $a's$ and $b's$ of length exactly three. $(a \cup b)(a \cup b)(a \cup b) = (a \cup b)^3$.

Example: $(a \cup b)^* a(a \cup b)^* a(a \cup b)^*$.

Example: $b^*ab^*a(a \cup b)^*$.

Example: $(a \cup b)^* ab^* ab^*$.

Theorem: For a formal language L, the following are equivalent:

1. L is regular.
2. L is denoted by a restricted regular expression.
3. L is denoted by a general regular expression.

Some languages are not regular. Take the next three examples.

Example: $\{a^n b^n | n \geq 0\}$.

Example: Any language in which parentheses are used in the usual way.

Example: $\{ww^R | w \in G^*\}$ where w^R is the reverse of w.

2.6.2 Pushdown Automata

This section describes "pushdown store" or a stack. There are languages which are not context-free. For example, $\{a^n b^n c^n | n \geq 0\}$. The languages can be recognized by Turing machines.

The following are equivalent:

1. Regular grammar.
2. Reverse regular grammar.
3. Transition graph.
4. State graph.
5. Finite automata (deterministic).

Corollary: If L is a language, the following are equivalent:

1. L is regular.
2. L is the language of a transition graph.

3. L is the language of a state graph.
4. L is the language of a finite automata.

If L_1 and L_2 are regular languages, then so are $L_1 \cup L_2$ and $L_1 \cap L_2$. Note that $G^* - L$ is the set of all strings over G which are not in L. This is called the complement of L. A two-way finite automata is an automaton which can move left and right on the input tape. Result: Every two way automaton has an equivalent one-way automaton. A two-way automation is not more powerful than a one-way finite automaton.

The test will cover ambiguous grammars (2 or more); grammars: what is regular. Draw transition and state graphs. Sets. Basic results in Chapter 9 in the textbook.

A *transition graph* is a state graph iff for every node and character in the alphabet, there is exactly one arc leaving that node labeled with that character. For example, for the input table,

$$\begin{array}{ccc} b & c & \\ \uparrow & \uparrow & \uparrow \\ S & S & Q \end{array}$$

R is called the *dead* or *trapped state.*

$$\begin{array}{cccc} c & c & b & c \\ \uparrow & \uparrow & \uparrow & \uparrow \\ S & Q & Q & R \end{array}$$

The last b is rejected because it is deterministic.

State graphs correspond to finite automaton. There is exactly one arc per character. See Figure 9.2.1 in the textbook. In a *non-deterministic finite automata,* t is not a function. (Q, b) may have more than one value or no value at all. If the input string is not accepted, we can not say it should be rejected. A different execution with the input string could lead to acceptance. Every transition graph can be seen as a non-deterministic finite automata. Every non-deterministic finite automata is equivalent to deterministic finite automata. Every transition graph can be converted to a state graph. The following is an algorithm to convert a transition graph into a state graph (version 2 only).

Step 1: Begin with state Q_1, which corresponds to the start node N_1. For each character of G, find the set of nodes to which there is an arc from N_1 labeled with that character. If this set consists of N_1 only, draw an arc from Q_1 to Q_1 labeled with the character, else add a new state Q_i and draw an arc from Q_1 to Q_i.

Step i : Check if there is an arc leaving each state node labeled with each character of G. If so, we are done. Else, if Q_i is a state node with no arc labeled "w" ($w \in G$) find the set of all nodes to which there is an arc labeled "w" from a node of Q_i. If there is already a state corresponding to this set, draw an arc from Q_i to that state node and label it "w" else add a new state node and draw an arc labeled "w" from Q_i to it.

Make a state an accepting state iff it corresponds to at least one accepting node in the transition graph.

Example: See Figure 2.10 for the transition graph. See Figure 2.11 for step 1. Many times state graphs can be simplified by collapsing several states into a single state. See Figure 2.12 for the collapsed graph.

Example: The following push down automata accepts the language $\{ww^r | w \in \{a, b\}^*\}$. $G = \{a, b\}$. $R = \{a, b\}$. $K = \{S, E\}$. $F = \{E\}$.

$t(S, a, b) = (S, a) =$ push "a"
$t(S, b, \lambda) = (S, b) =$ push "b"
$t(S, \lambda, \lambda) = (E, \lambda) =$ no read
$t(E, a, a) = (E, \lambda) =$ pop "a"
$t(E, b, b) = (E, \lambda) =$ pop "b"

This machine must guess when it has reached the middle of the input string and change from state S to state E in a non-deterministic way. Whenever the machine is in state S, it can choose to either push the next symbol onto the graph or to switch to state E.

$$\begin{array}{cccc} a & b & b & a \\ \uparrow & \uparrow & \uparrow & \uparrow \\ S & S & S & S \end{array}$$

Decision: can not accept the string, but not the same as reject.

$$\begin{array}{cccc} a & b & b & a \\ \uparrow & \uparrow & \uparrow & \uparrow \\ S & S & E & E \end{array}$$

Changes states only.

For homework, on page 247 in the textbook do problems 7, 9, 11, 13, 15. On page 320, do problems 1 thru 9.

The test will cover ambiguous grammars (2 or more); grammars: what is regular. Draw transition and state graphs. Sets. Basic results in Chapter 9 in the textbook.
A *transition graph* is a state graph iff for every node and character in the alphabet, there is exactly one arc leaving that node labeled with that character. For example, for the input table,

$$\begin{array}{ccc} b & c & \\ \uparrow & \uparrow & \uparrow \\ S & S & Q \end{array}$$

R is called the *dead* or *trapped state.*

$$\begin{array}{cccc} c & c & b & c \\ \uparrow & \uparrow & \uparrow & \uparrow \\ S & Q & Q & R \end{array}$$

The last b is rejected because it is deterministic. State graphs correspond to finite automaton. There is exactly one arc per character. See Figure 9.2.1 in the textbook. In a *non-deterministic finite automata, t* is not a function. (Q, b) may have more than one value or no value at all. If the input string is not accepted, we cannot say it should be rejected. A different execution with the input string could lead to acceptance.

Theorem: The class of languages accepted by push down automata is exactly the class of context-free languages.

There are languages that are not context-free. For example, $\{a^n b^n c^n | n \geq 0\}$. These languages can be recognized by Turing machines. Final results:

- Finite automata recognize regular languages.
- Push down automata recognize context-free languages.
- Turing machines can recognize all mu-recursive functions and recognize non-context free languages.

For homework, in Chapter 8 on page 247, do problems 7, 9, 11, 13, 15. In chapter 9 on page 308, do problems 11, 12, 13, 15. In Chapter 9 on page 320, do problems 1 thru 9. The final exam will be during Final Exam week.

2.7 Homework and Answers

Page 247 in the textbook.

Show that the grammar is ambiguous with two non-isomorphic derivation trees for the same string. Find an equivalent unambiguous grammar.

7.

$S \to bSE|\lambda$
$E \to bE|\lambda$

Solution: $\{b^n|n \neq 1\}$. $S \to bE|\lambda$. $E \to bE|\lambda$.

S
bSE
$bbSEE$
$bb\lambda EEbb\lambda bE$
$bb\lambda bb$
b^4

S
bSE
$b\lambda E$
$b\lambda bE$
$b\lambda bbE$
$b\lambda bbbb$
b^4

9. $S \to bSc|bSd|bS|\lambda$. Solution: Either $S \to bSc|bSd|H|\lambda$, $H \to bH|b$ or $S \to bSc|bSd|H$, $H \to bH|\lambda$.

S
bSc
$bbSdS$
$bbb\lambda dc$
b^3dc

S
bS
$bbSc$
$bbbSdc$
$bbb\lambda dc$
b^3dc

11.

$S \to cS|cSb|Q$
$Q \to cQc|c$

Solution: $\{c^nb^m|m \geq 0, n \geq 1, n \leq m\}$. $S \to cSb|Q$. $Q \to cQ|c$.

S
cS
ccS
ccQ
ccc
c^3

S
Q
cQc
ccc
c^3

13.

$S \to bSE|\lambda$
$E \to cE|c$

Solution: $S \to bSc|bHc|\lambda$. $H \to cH|c$.

S
bSE
$bbSEE$
$bb\lambda EE$
$bb\lambda cEE$
$bb\lambda ccE$
$bb\lambda ccc$
b^2c^3

S
bSE
$bbSEE$
$bb\lambda EE$
$bb\lambda cE$
$bb\lambda ccE$
$bb\lambda ccc$
b^2c^3

15.

$S \to bS|bE$
$E \to Ed|Fd$
$F \to bFd|bddd$

Solution: $\{b^n d^m | n \geq 2, m \geq 4\}$. $S \to bS|bE$. $E \to Ed|Fd$. $F \to bddd$.

S
bE
bEd
$bEdd$
$bEddd$
$bbFdddd$
$bbbddddddd$
b^3d^7

S
bS
bbE
$bbEd$
$bbEdd$
$bbEddd$
$bbFdddd$
$bbbddddddd$
b^3d^7

The final exam is on Thursday afternoon from 12:30 to 2:30pm.

2.8 Homework and Answers

Problems on page 308 in the textbook. Do # 11, 12, 13, 15.

In Exercises 1 to 22, draw a transition graph for each set.

11. The set of strings over $\{b, c\}$ whose length is no greater than 5. Solution: See Figure 2.13.
12. The set of strings over $\{b, c\}$ whose length is at least 5. Solution: See Figure 2.14.
13. The set of all strings over $\{b, c\}$ with length at least two, having an even number (possibly zero) of $b's$. Solution: See Figure 2.15.

2.9 Homework and Answers

Problems on page 320 in the textbook.

1. Convert Figures 9.1.1, 9.1.3 to 9.1.7 and 9.1.9 to 9.1.11, respectively, into equivalent state graphs. Solution: Figure 2.16 gives the state graph for Figure 9.1.1. Figure 2.17 gives the state graph for Figure 9.1.3. Figure 2.18 gives the state graph for Figure 9.1.7 in the textbook. Figure 2.19 gives the state graph for Figure 9.1.9 in the textbook.

2.10 Handout and Answers

1. Give a regular expression for each of the following languages over the alphabet $\{a, b\}$.

   a. All strings which at some point contain a double letter (aa or bb). Solution: $G = \{a, b\}$. $(a \cup b)^*(aa \cup bb)(a \cup b)^*$.

   b. All strings which do not contain a double letter. Solution: $(a \cup b)^* - (a \cup b)^*(aa \cup bb)(a \cup b)^*$. Alternatively, $(ab)^* = \{\lambda, ab, abab, ababab, ...\}$. $(\Lambda \cup b)(ab)^*(a \cup \Lambda)$.

   c. All strings containing exactly three $b's$. Solution: $a^*ba^*ba^*ba^*$.

   d. All strings that contain the substring aaa or the substring bbb but not both. Solution: $(a \cup b)^*(aa \cup bb)$.

2. Describe the languages of the following regular expressions.

   a. $(a^*b^*)^*$.

   b. $b^*(abb^*)(\Lambda \cup a)$. Solution: Two $a's$ not adjacent. Has ab.

   c. $(ab)^*a$. Solution: It has to end in a. λ is not in the set.

   d. $a(aa)^*(\Lambda \cup a)b \cup b$. Solution: a^*b.

   e. $(a \cup b)^*a(\Lambda \cup bbbb)$. Solution: It has at least one a. Can end in a or $bbbb$. Can only be a.

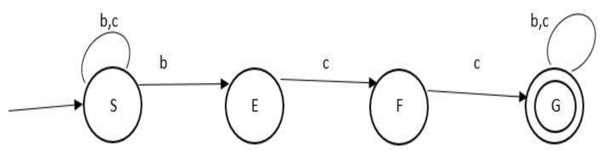


Figure 2.10: This figure shows the transition graph that needs to be simplified

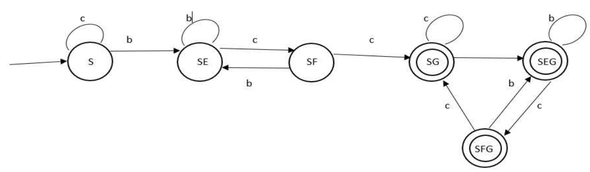


Figure 2.11: This figure shows step 1 of the simplified transition graph

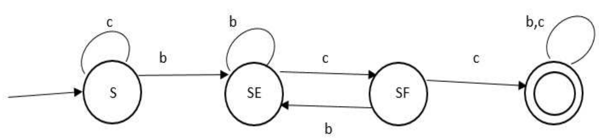


Figure 2.12: This figure shows the final step of the simplified transition graph

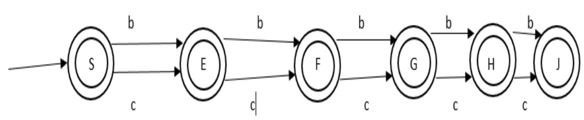


Figure 2.13: This figure shows the solution to problem 11 on page 308 in the textbook

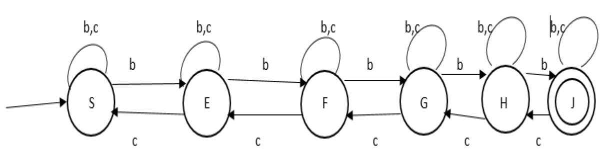


Figure 2.14: This figure shows the solution to problem 12 on page 308 in the textbook

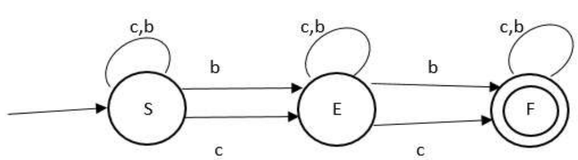


Figure 2.15: This figure shows the solution to problem 13 on page 308 in the textbook

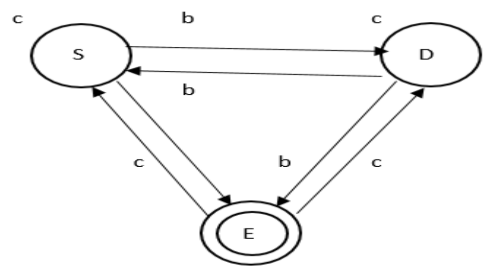


Figure 2.16: This figure shows the state graph for Figure 9.1.1 to problem 1 on page 320 in the textbook

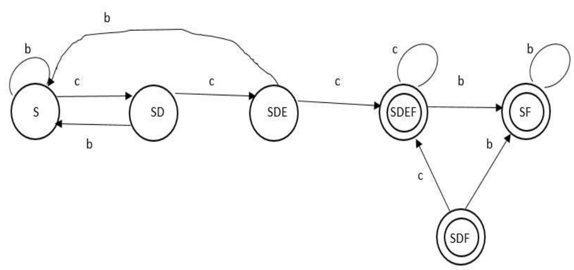


Figure 2.17: This figure shows the state graph for Figure 9.1.3 to problem 1 on page 320 in the textbook

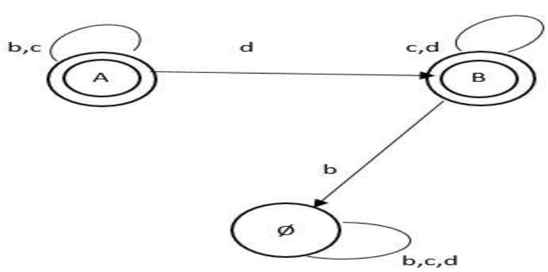


Figure 2.18: This figure shows the state graph for Figure 9.1.7 to problem 1 on page 320 in the textbook

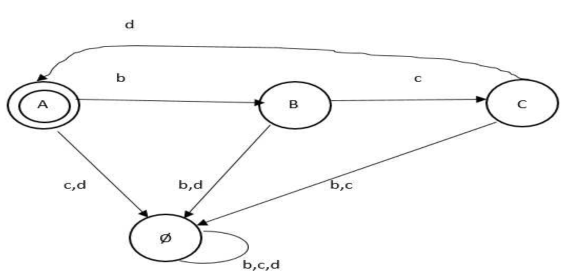


Figure 2.19: This figure shows the state graph for Figure 9.1.9 to problem 1 on page 320 in the textbook

Chapter 3

Vector Processing and Supercomputers

Course: CSCI 584
Place: College of William and Mary
Instructor: J. J. Lambiotte
Timeframe: Fall 1992
Phone: 864-5794, Home: 886-0053

Grading
Homework 10%
Programs 40%
Paper 20%
Exam 30%

Notes:

1. "Supercomputing" paper due approximately Dec. 1, 1992
2. Two or three programs
3. Final exam take-home — may include programming problem
4. E-mail lambj@jaysum.larc.nasa.gov

Course Summary

Three Paths:

1. Supercomputing concepts (General)

    Scalar vs vector vs parallel

    Performance measures

    Algorithms

    - Linear equations
    - Matrix multiplication
    - Finite differences

2. Supercomputer Specific

- CYBER-205
- CRAY-2, CRAY Y-MP
  - Architecture, performance
  - Algorithms

3. Programming Experience

   - Voyager, Sabre

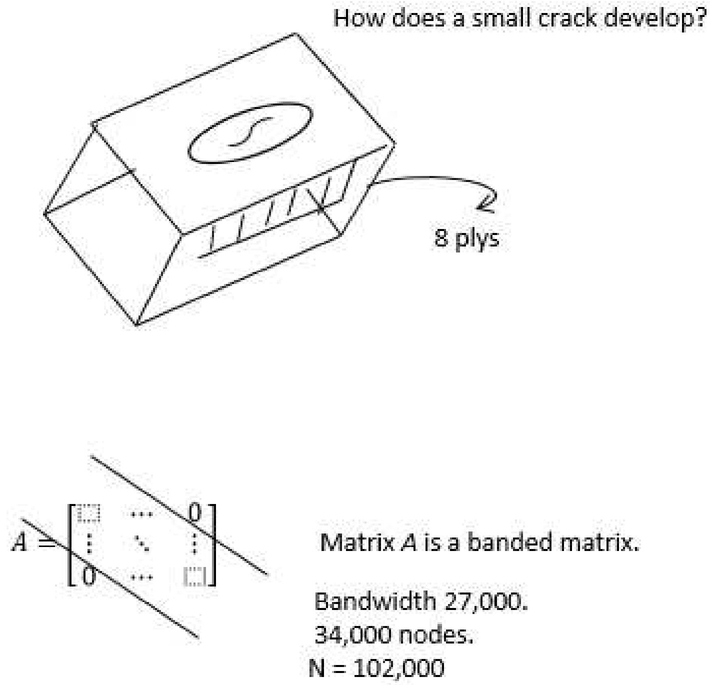


Figure 3.1: This figure shows the example of solving the problem of a small crack in composite material

3.1 Introduction

A *supercomputer* is one of a small group of computers accepted to be significantly more powerful than the vast majority of scientific computers. Supercomputers are characterized by four things:

1. Large, but fast memory.
2. Extraordinarily fast CPU's.
3. Non-conventional architectures.
4. Expensive machines.

Supercomputers are used to solve problems that cannot be solved using a workstation. Take for example the composite material research problem on the Cyber 205. See Figure 3.1. How does a small crack develop? Solve the symmetric system of equations $A\,x = b$ where A is a positive definite matrix. An algorithm is

1 [**For** i = 1, n
  2 [At the i^{th} step
    Form L_i
    For j = i+1, i+2, ..., i+b
    [Add multiples of L_i to j^{th} column

It took 1.3 hours at 156 million floating-point operations per second, called *megaflops,* to solve the problem. There are three major ingredients:

1. CPU power (65 hours of Cyber 175).

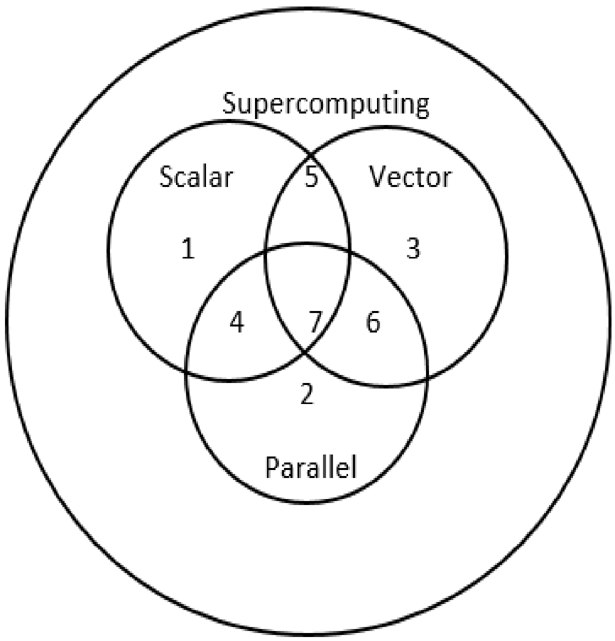


Figure 3.2: This figure shows an overview of supercomputing

2. Memory $= S = N\beta = 270$ Mwords.
   - Virtual memory machine.
   - 8 Mwords of real memory (64 bits per word).
3. Unique architecture.
   (a) Column multiplication.
   (b) Must deal with thrashing.

See Figure 3.2.

1. Conventional serial computers — Cyber 180.
2. CM-2 (thinking machines) — every processor does the exact same thing.
3. Empty ($\emptyset$) — most have a scalar unit.
4. Intel IPSC/860 — independent processors.
5. Cyber-205, CRAY-1
6. Empty ($\emptyset$)
7. CRAY XMP, YMP, CRAY-2, CM-5 — have vectored units that can operate in parallel and scalar units that can operate in parallel.

Mflops means millions of floating-point operations per second. *Stride* refers to the ways vectors are arranged in memory. *Register to registers* are downloads of vectors to registers to do computations and store in memory (CRAY-YMP).

3.2 Vectorizable Task

The following statements characterize a vectorizable task.

1. *Repeated* computation on a *large* set of data.

   (a) $c_i = a_i + b_i$, $i = 1, ..., 1000$.

   (b) $c_i = (a_i + b_i - 3)/(e_i * e_i)$, $i = 1, ..., 1000$.

   (c) Solve 1000 independent sets of tridiagonal equations.

2. Source and result operands must be independent.

```
  DO 2 j = 2, N-1
  DO 1 i = 2, N-1
1    A(i,j) = B(i,j) - A(i, j-1) * C(i,j) 'yes, vectorizable
     A(i,j) = B(i,j) - A(i-1, j) * C(i,j) 'no, not vectorizable
     A(i,j) = B(i,j) - A(i+1, j) * C(i,j) 'yes, vvectorizable
```

3. Must be able to store the data as a vector. Best performance implies:

   (a) Computations are over contiguous locations (or odd strides) — innermost loop is over the first dimension and there is little or no indirect addressing (e.g. $A(I(j)) = \cdots$).

   (b) The data is referenced in only one direction — data referenced in multiple directions can be a problem.

3.2.1 Taylor's Theorem

$$U'(x) = \lim_{h \to 0} \frac{U(x+h) - U(x)}{h}.$$

Taylor's Theorem: if U is a function with $n+1$ derivatives existing everywhere in some interval I, and if x and $x+h$ are two points in I, then there exists a value z between x and $x+h$, $z \in (x, x+h)$, such that

$$U(x+h) = U(x) + hU'(x) + \frac{h^2}{2}U''(x) + \cdots + \frac{h^n}{n!}U^n(x) + \frac{U^{n+1}(z)}{(n+1)!}.$$

The first order approximation to $U(x)$ is

$$U(x+h) = U(x) + hU'(x) + \frac{h^2 U''(z)}{2!}, \quad z \in (x, x+h)$$

where

$$U'(x) = U(x+h) - U(x) - \frac{h^2 U''(z)}{2!} = \frac{U(x+h) - U(x)}{h} + e.$$

$$U'(x) \approx \frac{U(x+h) - U(x)}{h}.$$

Say, $|U''(x)| \leq m$ for all $x \in I$. Then,

$$\left| U'(x) - \frac{U(x+h) - U(x)}{h} \right| \leq \frac{nm}{2}.$$

A second order approximation is

$$U(x+h) = U(x) + hU'(x) + \frac{h^2 U''(x)}{2!} + \frac{h^3 U'''(z_1)}{3!},$$

$$U(x-h) = U(x) - hU'(x) + \frac{h^2 U''(x)}{2!} - \frac{h^3 U'''(z_2)}{6},$$

$$U(x+h) - U(x-h) = 2hU'(x) + \frac{h^3}{6}\left[U'''(z_1) + U'''(z_2)\right].$$

$$U'(x) = \frac{U(x+h) - U(x-h)}{2h} - \frac{h^2}{12}\left[U'''(z_1) + U'''(z_2)\right].$$

$$U'(x) \approx \frac{U(x+h) - U(x-h)}{2h},$$

$$e = \frac{h^2}{6} m \Rightarrow \bigcirc(h^2).$$

To derive an approximation for $U''(x)$:

$$U(x+h) + U(x-h) = 2U(x) + h^2 U''(x) + \frac{h^4}{24}\left[U^4(z_1) + U^4(z_2)\right],$$

$$U''(x) = \frac{U(x-h) - 2U(x) + U(x+h)}{h^2} - \frac{h^2}{24}\left[U^4(z_1) + U^4(z_2)\right].$$

Solutions

To solve $U''(x) = f(x)$ on the line (a, b), $U(0) = a$ and $U(1) = b$, we can use finite differences. Choose n points on a line.

```
|----|----|----|----|----|----|-----|----|
                                         n = 9
x=0                                      x = 1
```

$$h = \frac{1}{n-1},$$

$$x_i = (i-1)h,$$

$$U(x_i) = U_i,$$

$$f(x_i) = f_i,$$

Then,

$$\frac{U_{i-1} - 2U_i + U_{i+1}}{h^2} = f_i, \text{ at } i = 2 \text{ to } n-1.$$

$$U_i = 0.5(-h^2 f_i + U_{i-1} + U_{i+1}).$$

Jacobi (use old values):

$$U_I^{(k)} = 0.5(-h^2 f_i + U_{i-1}^{k-1} + U_{i+1}^{k-1})$$

Gauss-Seidel (use latest available information):

$$U_i^{(k)} = 0.5(-h^2 f_i + U_{i-1}^{k} + U_{i+1}^{k-1})$$

Gauss-Seidel converges twice as fast.

$$U^{(0)}(x) = 0.$$

Show $U(x,y)$ where U_{xx} and U_{yy} are partial derivatives.

$$U_{xx} + U_{yy} = U(x+h,y) + U(x-h,y) - 4U(x,y) + \frac{U(x,y+h) + U(x,y-h)}{h^2} + e, \;\; e = \bigcirc(h^2).$$

Hint: Using Taylor's Theorem,

$$U(x+h,y) = U(x,y) + hU_x(x,y) + \frac{h^2}{2}U_{xx}(x,y) + \frac{h^3}{6}U_{xxx}(x,y) + \frac{h^4}{4!}U_{xxxx}(\xi,y), \text{ where } \xi \in (x, x+h).$$

We need the above result for Programming Assignment 1.

Cyber 205

6-bits. $C = A + B$.

```
----------------------------------------
| OP | 6-bit | A | --- | B | Z | C | X |
----------------------------------------

256 registers. The descriptor is:

0    15    63
------------
| LT | FWA |
------------
```

G-bit (0-7):

0 — On— 64 bit arithmetic. Off — 32-bit.

1 — On — control vector operates on 1's. Off — control vector operates on 0's.

3 — On — A is a broadcast (not a vector).

5,6,7 — Sign control. 10x — use magnitude of elements of A. 11x — make all positive elements negative in A.

Example: Compare $Z(1;N) = A(1;N).LT.B(1;N)$.

$$\begin{array}{c}A\\ \begin{bmatrix}4\\3\\6\\2\\9\end{bmatrix}\end{array}\begin{array}{c}B\\ \begin{bmatrix}5\\-1\\4\\6\\15\end{bmatrix}\end{array}\rightarrow\begin{array}{c}Z\\ \begin{bmatrix}1\\0\\0\\1\\1\end{bmatrix}\end{array}\rightarrow\begin{bmatrix}5\\6\\15\end{bmatrix}$$

To obtain the final vector with 3 elements, it is $A = B$ compressed by Z. $A(1;num) = Q8CMPRS(B(1;N), Z(1;N), A(1;num))$.

Example: $C = A$ merge B by Z, where $0 =$ use right and $1 =$ use left.

$$\begin{bmatrix}2\\6\\3\end{bmatrix}\begin{bmatrix}3\\1\\9\end{bmatrix}\text{ by Z}\begin{bmatrix}1\\1\\0\\0\\0\\1\end{bmatrix}\rightarrow\begin{bmatrix}2\\6\\5\\1\\9\\3\end{bmatrix}$$

Vector Macros

Here are some definitions for vector macros:

1. The adjacent mean $c_j = \frac{a_{j+1}+a_j}{2}$.
2. The average $c_j = \frac{a_j+b_j}{2}$.
3. The delta $c_j = A_{j+1} - A_j$.

Example: $S = Q8SDOT(A(1;N), B(1;N))$.

$$\begin{bmatrix}a_1\\a_2\\\vdots\\a_n\end{bmatrix}\rightarrow\begin{bmatrix}a_n\\a_{n-1}\\\vdots\\a_2\\a_1\end{bmatrix}$$

reverses the vectors.

Example: $B = [101, 102, 103, 104]$. $I = [2, 3, 1, 4]$. Scatter $B \rightarrow C$ using I. $C = [103, 101, 102, 104]$. Gather $B \rightarrow C$ using I. $C = [102, 103, 101, 104]$.

A control store looks like:

```
-----0----0----0----0----0------
|    |    |    |    |    |     |
|    .    |    |    |    |     |
|    |    |    |    |    |     |
|    |   \./   |    |    |     |
|    |    |    |    |    |     |
|    |    |    |   \./   |     |
|    |    |   \./   |    |     |
|   \|/   |    |    |   \|/    |
-----0---------0---------0------
```

A bit-vector looks like:

```
-----0----0----0----0----0------
|    |    |    |    |    |     |
|    *    |    |    |    |     |
|    |    |    |    |    |     |
|    |    *    |    |    |     |
|    |    |    |    |    |     |
|    |    |    |    *    |     |
|    |    |    *    |    |     |
|    |    |    |    |    |     |
-----0----0----0----0----0------
```

Consider the computation $a_{ij} = b_i - b_{ij-1}$ which is at the interior. The term a_{ij} is at the boundary.

Example: $LT = N{*}M{-}2{*}N{-}2$. $T(2,2;LT) = B(2,2;LT){-}B(2,1;LT)$. $A(2,2;LT) = Q8KTRL(T(2,2;LT)$, $BT(2,2;LT), A(2,2;LT))$ where $BT(2,2;LT)$ $A(2,2;LT) = B(2,2;LT) - B(2,1;LT)$.

3.2.2 Homework

Problem 1: Use Jacobi and Gauss-Seidel methods to solve as efficiently as possible the following PDE: $U_{xx} + U_{yy} = f(x, y, U)$ at the interior points and with the boundary conditions:

$$\begin{array}{ll} U(0,y) = 0, & U(1,y) = y^4 - y - 3 \\ U(x,0) = -3x^2, & U(x,1) = x - 4x^2 \end{array}$$

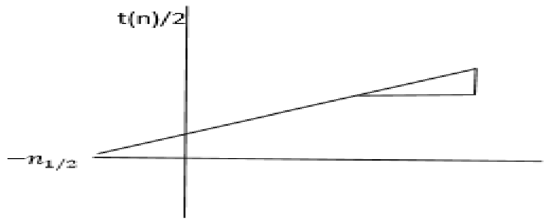
where $f(x,y,U) = 12y^2x - 2(y+3)U(x,y)$ and $U(x,y) = U((i-1)h,(j-1)h) \doteq U_{ij}$. Develop the equations specifically for $n = 32$ ($h = 1/31$). Using $U^0(x,y) = xy$ at the interior as the initial estimate, consider the solution converged when:

$$\max_{i,j}\left|\frac{U_{ij}^k - U_{ij}^{k-1}}{U_{ij}^{k-1}}\right| < \epsilon$$

where $\epsilon = 10^{-6}$.

Programming notes:

1. Put an iteration limit of 5,000 in the program.
2. In computing $f(x, y, U)$, use the old value for U in both algorithms.
3. At convergence, print out:
   (a) Maximum error.
   (b) U_{ii} for $i = 1, 32$ (6F13.6 format) and $\sum_{i=1}^{32} U_{ii}$ and sum the 32 numbers.
   (c) The total CPU time and time per iteration for each algorithm where the CPU time includes only the iteration step (not the error calculation or the initialization).
4. Vectorize to the fullest extent.
5. Run on both Voyager and Sabre, and then turn in a listing of your programs and output along with a description of the problem and analysis of the results. Which ran faster? Why?
6. The exercise is due October 19, 1992.



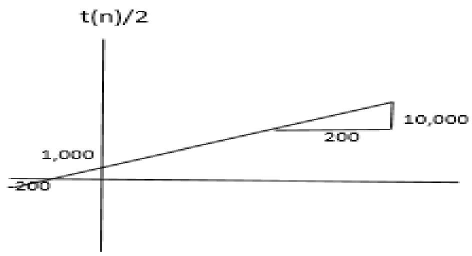


Figure 3.3: This figure shows two graphs of the problem size n versus the timing $t(n)$.

Solution Timing

1. $F(n) = f(n)\bar{n} = 4n(\frac{2}{3}n)$.

$T(n) = 2n\tau(52 + \frac{\bar{n}}{4}) + \tau n(116 + \bar{n}) =$

$\tau n(104 + \frac{\bar{n}}{2} + 116 + \bar{n}) =$

$\tau n(220 + \frac{2}{3}\bar{n}) =$

$\frac{3}{2}n\tau(146 + \bar{n}) =$

$(4n)\frac{3}{8}\tau(146 + \bar{n}) \Rightarrow$

$r_\infty = \frac{1}{\tau\alpha} = \frac{8}{3}(50) = 133,$

where $\bar{n}_{\frac{1}{2}} = 146 \Rightarrow n_{\frac{1}{2}} = \frac{3}{2}(146) = 216.$

2. For $F(n) = 2n,:$

n	$t(n)$ nsecs	$\frac{t(n)}{2}$
100	2660	1330
300	4660	2330

$t(n) = \alpha m\tau(C + n)$. $\frac{t(n)}{m} = \alpha\tau(C + n) = r_\infty^{-1}(C + n)$. $C = n_{\frac{1}{2}}$. See Figure 3.3. It shows two graphs of the problem size n versus the timing $t(n)$. $r_\infty = \frac{200}{10000 \times 10^{-9}} = 200$ mflops. $C = A + BS \Rightarrow F(n) = 2n$.

Instruction	Issue	First Result	Last Result
Load B	0	35	34 + L
Load A	34+L	69+L	68+2L
Multiply B*S	35+L	58+L	57+2L
Add A+B*S	68+2L	91+2L	90+3L
Store C	90+3L	125+3L	124+4L

On the Cray-2, $T = \tau(LSU + \frac{n}{64}(124 + 4(64))) = \tau(LSU + 6n) = 6\tau(\frac{LSU}{6} + n) = 2(3)\tau(\frac{LSU}{6} + n) \Rightarrow r_\infty = \frac{1}{\tau\alpha} = \frac{1}{3}(240) = 80$ mflops on the Cray-2. $n_{\frac{1}{2}} = \frac{400}{6}$.

On the Cray-YMP with chaining and piping,

Instruction	Issue	First Result	Last Result	Comment
Load B	0	20	19 + L	2 load pipes
Load A	1	21	20+L	2 load pipes
Multiply B*S	20	33	32+L	chaining
Add A+B*S	33	45	44+L	chaining
Store C	45	65	64+L	store pipe

$T = \tau(LSU + \frac{n}{64}(64 + 1 * 64)) = \tau(LSU + 2n) = 2\tau(\frac{LSU}{2} + n) = 2(1)\tau(200 + n) \Rightarrow n_{\frac{1}{2}} = 200$, $r_\infty = \frac{1}{\tau\alpha} = (1)(166) = 166$ mflops.

A tri-diagonal matrix set-up looks like this $Dx = B$:

$$\overset{D}{\begin{bmatrix} \ddots & & & \\ & \ddots & & \\ & & \ddots & \\ & & & \ddots \end{bmatrix}} \overset{x}{\begin{bmatrix} \\ \\ \\ \end{bmatrix}} = \overset{B}{\begin{bmatrix} \\ \\ \\ \end{bmatrix}}$$

Dim D(N), X(N), B(N). B(1; N) = D(1; N) * X(1; N).

A four-diagonal matrix looks like this $Ax = B$:

$$\overset{A}{\begin{bmatrix} x_{11} & x_{14} & & \\ & \ddots & \ddots & 0 \\ & & \ddots & \ddots \\ & 0 & & \ddots \end{bmatrix}} \overset{x}{\begin{bmatrix} \\ \\ \\ \end{bmatrix}} = \overset{B}{\begin{bmatrix} \\ \\ \\ \end{bmatrix}}$$

where

$$\begin{bmatrix} b_1 \\ b_2 \\ \downarrow \\ b_n \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{22} \\ \downarrow \\ a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \downarrow \\ x_n \end{bmatrix} + \begin{bmatrix} a_{14} \\ a_{25} \\ \downarrow \\ a_{n-3,n} \end{bmatrix} \begin{bmatrix} x_4 \\ x_5 \\ \downarrow \\ x_n \end{bmatrix}$$

D(n,2). b(1; n) = D(1, 1; N)*X(1; N). b(1; n-3) = D(1, 2; N-3) * x(4; N-3) + b(1; N - 3).

Solution Iterative Methods

Solve $Au = b$. Write $A = L + D + R$ where L equals to a strictly lower diagonal matrix, D equals to a main diagonal matrix, and R equals to a strictly upper diagonal matrix. The Jacobi equation is $DU^{k+1} = (-L - R)U^k + b \Rightarrow U^{k+1} = D^{-1}[-L - R)U^k + b]$. The Gauss-Seidel equation is $(L+D)U^{k+1} = -RU^k + b \Rightarrow U^{k+1} =$

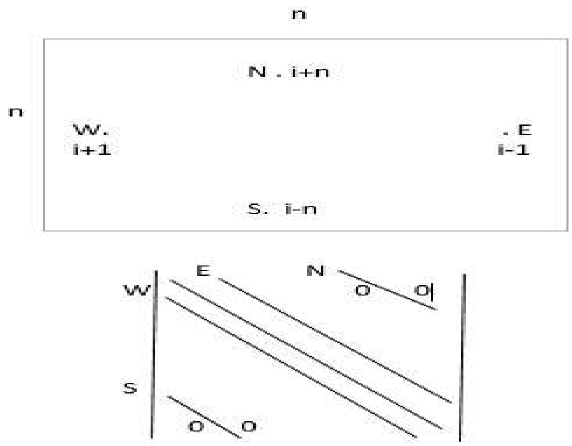


Figure 3.4: This figure shows a conceptual view of the Poisson equations.

$(L+D)^{-1}[-RU^k+b]$. The Poisson equation is $U_{xx}+U_{yy} = f(x,y)$. $U_{i-n}+U_{i-1}-4U_i+U_{i+1}+U_{i+n} = h^2 f_i$. See Figure 3.4.

$$A = \left[\begin{array}{c|c|c|c|c} C & I & & & \\ \hline I & C & I & & \\ \hline & I & C & I & \\ \hline & & & & I \\ \hline & & & I & C \end{array}\right].$$

$$C = \begin{bmatrix} -4 & 1 & & & & & \\ 1 & -4 & 1 & & & & \\ & 1 & -4 & 1 & & & \\ & & 1 & -4 & 1 & & \\ & & \ddots & \ddots & \ddots & & \\ & & & 1 & -4 & 1 \\ & & & & 1 & -4 \end{bmatrix}.$$

For the Jacobi method, $U^{k+1} = D^{-1}[-LU^k - RU^k + b]$ where D^{-1} is just another diagonal matrix. $D = -4I \Rightarrow D^{-1} = -\frac{1}{4}I$. $-L, -R$ are diagonally stripped. Therefore, $\bigcirc(n^2)$. Store as $coeffs(N,N,5)$ or as $(N*N,5)$.

For the Gauss-Seidel method, $(L+D)U^{k+1} = -RU^k + b = r$. $r_i = U_{i+1}^k + U_{i+n}^k + h^2 f_i$.

$$\begin{bmatrix} D_1 & 0 & & & \\ L_2 & D_2 & & & \\ & L_3 & D_3 & & \\ & & \ddots & \ddots & \\ & & & L_n & D_n \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ \vdots \\ U_n \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ \vdots \\ r_n \end{bmatrix},$$

where $L_i = I$. $D_1 U_1^{k+1} = r_1 \Rightarrow U_1^{k+1} = D_1^{-1} r_1$. $L_2 U_1^{k+1} + D_2 U_2^{k+1} = r_2 \Rightarrow D_2 U_2^{k+1} = r_2 - L_2 U_1^{k+1}$. $U_2^{k+1} = D_2^{-1}[r_2 - L_2 U_1^{k+1}]$. So,

$$\begin{bmatrix} -4 & & \\ 1 & -4 & \\ & 1 & -4 \end{bmatrix} \begin{bmatrix} U_1^{k+1} \\ U_2^{k+1} \\ U_3^{k+1} \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix}.$$

$U_1^{k+1} = \frac{r_1}{-4}$. $-4U_2^{k+1} = r_2 - U_1^{k+1}$. $U_2^{k+1} = -\frac{1}{4}(r_2 - U_1^{k+1})$. $r \leftarrow RU^k + b \Rightarrow \bigcirc(n^2)$. $r_2 - L_2U_1^{k+1} \Rightarrow \bigcirc(n)$. $D_2U_2^{k+1}$ equals to the recursive part which is also the right-hand side.

Red and Black or Checker Board Ordering

Consider the grid:

```
 0      0      0      0      0      0      0
22     47     23     48     24     49     25

                                 -------
 0      0      0      0      0  |   0  |   0
43     19     44     20     45  |  21  |  46
                                |      |
                          -------      ------
 0      0      0      0  |   0      0      0 |
15     46     16     41  |  17     42     18 |
                         |                   |
                          ------       ------
 0      0      0      0      0  |   0  |   0
36     12     37     13     38  |  14  |  39
                                 -------
                    -------
 0      0      0  |   0  |   0      0      0
 8     33      9  |  34  |  10     35     11
              -------      -------
 0      0  |   0      0      0  |   0      0
29      5  |  30      6     31  |   7     32
              -------      -------
 0      0      0  |   0  |   0      0      0
 1     26      2  |  27  |   3     28      4
                    -------
```

$$\begin{array}{c} \frac{n^2}{2} \\ \frac{n^2}{2} \end{array} \left[\begin{array}{c|c} x & x \\ \hline x & x \end{array}\right]$$

$(L+D)U^{k+1} = -RU^k + b$ has the matrix form:

$$\left[\begin{array}{c|c} D_1 & 0 \\ \hline L_2 & D_2 \end{array}\right] \left[\begin{array}{c} U_1^{k+1} \\ \hline U_2^{k+1} \end{array}\right] = \left[\begin{array}{c} r_1 \\ \hline r_2 \end{array}\right].$$

$D_1U_1^{k+1} = r_1 \Rightarrow U_1^{k+1} = D_1^{-1}r_1$. $D_2U_2^{k+1} = r_2 - L_2U_1^{k+1}$. $U_2^{k+1} = D_2^{-1}[r_2 - L_2U_1^{k+1}]$. All vectors vectorize in the Gauss-Seidel method. The convergence rate is slower.

An alterate ordering to improve convergence is to do a diagonal ordering.

$$\begin{bmatrix} \cdot & & & & & & \\ \cdot & & & & & & \\ \cdot & & & & & & \\ 16 & & & & & & \\ 11 & 17 & & & & & \\ 7 & 12 & 18 & & & & \\ 4 & 8 & 13 & 19 & & & \\ 2 & 5 & 9 & 14 & 20 & & \\ 1 & 3 & 6 & 10 & 15 & 21 & \dots \end{bmatrix}$$

$L + D + R$. $U_1^{k+1} = D_1^{-1} r_i \Rightarrow \bigcirc(\frac{n}{2})$. $D_2 U_2^{k+1} = r_2 - L_2 U_1^{k+1}$, and so on to U_n^{k+1}.

Fortran Code

This is the FORTRAN 77 code on the CRAY for the Jacobi matrix.

```
parameter (n = 32, h = 1./(n-1), eps = 1.e-6, itmax = 8000)
dimension uold(n, n), u(n, n), hf(n, n)
hsq = h*h
    do 2 j = 1, n
    y = (j-1)*h
        do 1 i = 1, n
        x = (i-1.) * h
        uold(i, j) = x * y
        1 continue
    uold(n, j) = y*y*y*y - y - 3.
    2 continue
    do 3 i = 1, n
    x = (i - 1)*h
    uold(i, 1) = -3.*x*x
    uold(i, n) = x - 4.*x*x
    3 continue
c write (6, 10) uold
101 format (8e12.4)
```

```
  c begin iteration
  cpu = 0.
  numits = 0
  200 continue
  t1 = second()
  numits = numits + 1
  if (numits .gt. itmax) stop
    do 15 j = 2, n-1
    y = (j-1)*h
    ysq = y*y
      do 15 i = 2, n-1
      x = (i-1)*h
6     hf(i, j) = -hsq*(12.*ysq*x - 2.*(y + 3.)*uold(i, j))
1     u(i, j) = .25*(hf(i, j) + uold(i, j-1) + uold(i, j+1) + uold(i+1, j) + uold(i-1, j))
      15 continue
    cpu = cpu + second() - t1
    num = 0
5   diffmax = 0.
      do 7 j = 2, n-1
        do 6 i = 2, n-1
        diff = (u(i, j) - uold(i, j)) / uold(i, j)
        diff = abs(diff)
7 8     uold(i, j) = u(i, j)
        if (diff .gt. diffmax) diffmax = diff
        if (diff .gt. eps) num = num + 1
        6 continue
      7 continue
```

```
  if (mod(numits, 100) .eq. 1) write (6, 100) num, diffmax
  100 format (/i5, e12.4)
  c stop
  if (num .gt. 0) go to 200
  write (6, 110) numits
  ave = cpu / numits
1 write(6, 115) cpu, ave
  115 format (/' total time, time per iteration ', 2e12.4/)
  write (6, 101) uold
  call check (uold, n, h)
  stop
  110 format (////' convergence, its = ',i6///)
  end
```

This is the FORTRAN 77 code on the CRAY for the Gauss-Seidel matrix.

```
parameter (n = 32, h= 1./(n-1), eps = 1.e-6, itmax = 5000)
dimension uold(n, n), u(n, n), hf(n, n)
hsq = h*h
    do 2 j = 1, n
    y = (j-1)*h
        do 1 i = 1, n
        x = (i-1)*h
        uold(i, j) = x*y
        1 continue
    uold(n, j) = y*y*y*y - y - 3.
    uold(1, j) = 0.
    u(n, j) = uold(n, j)
    u(1, j) = 0
    2 continue

    do 3 i = 1, n
    x = (i-1)*h
    uold(i, 1) = -3.*x*x
    uold(i, n) = x - 4.*x*x
    u(i, 1) = uold(i, 1)
    u(i, n) = uold(i, n)
    3 continue
write(6, 101) uold
101 format (8e12.4)

c begin iteration
cpu = 0.
numits = 0.
200 continue
t1 = second()
numits = numits+1
if (numits .gt. itmax) stop
    do 15 j = 2, n-1
    y = (j - 1)*h
    ysq = y*y
        do 15 i = 2, n-1
        x = (i-1)*h
        hf(i, j) = -hsq*(12. * ysq*x - 2.*(y + 3.)*uold(i, j))
        u(i, j) = .25*(hf(i, j) + u(i, j-1) + uold(i, j+1) + uold(i+1, j) + u(i-1, j))
        15 continue
    cpu = cpu + second() - t1
    num = 0
    diffmax = 0.
        do 7 j = 2, n-1
            do 6 i = 2, n-1
            diff = (u(i, j) - uold(i, j)) / uold(i, j)
            diff = abs(diff)
            uold(i, j) = u(i, j)
            if (diff .gt.diffmax) diffmax = diff
            if (diff .gt.eps) num = num + 1
            6 continue
        7 continue
```

```
     if (mod(numits, 100) .eq. 1) write (6, 100) num, diffmax
     100 format (/15, e12.4)
1    c stop
     if (num .gt. 0) go to 200
     write (6, 110) numits
     ave = cpu/numits
```

This is the modified and vectored Fortran 77 code for the Gauss-Seidel matrix.

```
     parameter (n = 32, h = 1./(n-1), eps = 1.e-6, itmax = 5000)
     dimension uold(n, n) u(n, n) hf(n, n)
     dimension t(n)
     hsq = h*h
        do 2 j = 1, n
        y = (j - 1)*h
           do 1 i = 1, n
1          x = (i - 1)*h
        3  uold(i, j) = x*y
     2     1 continue
        uold(n, j) = y*y*y*y - y - 3.
        uold(1, j) = 0.
        u(n, j) = uold(n, j)
        u(1, j) = 0.
        2 continue
```

```
        do 3 i = 1, n
        x = (i - 1) * h
        uold(i, 1) = -3.*x*x
     4  uold(i, n) = x - 4.*x*x
1       u(i,1) = uold(i, 1)
        u(i, n) = uold(i, n)
        3 continue
     c write (6, 101) uold
     101 format (8e12.4)
```

```
      c
      c
      c begin iteration
      c
      cpu = 0.
      numits = 0
      200 continue
      t1 = second()
      numits = numits + 1
      if (numits .gt. itmax) stop
         do 15 j = 2, n-1
1        y = (j - 1)*h
         ysq = y*y
            do 14 i = 2, n-1
            x = (i-1)*h
   6        hf(i, j) = -hsq*(12.*ysq*x - 2.*(y + 3.)*uold(i, j))
5           t(i) = hf(i, j) + u(i, j-1) + uold(i, j+1) + uold(i+1, j)
            14 continue
         c do the scalar part separately
            do 40 i = 2, n-1
   7        u(i, j) = .25*( t(i) + u(i-1, j))
            40 continue
         15 continue
      cpu = cpu + second() - t1
```

```
      num = 0
      diffmax = 0.
         do 7 j = 2, n-1
            do 6 i = 2, n-1
1           diff = ( u(i, j) - uold(i, j) / uold(i, j)
8           diff = abs(diff)
   9        uold(i, j) = u(i, j)
            if (diff .gt. diffmax) diffmax = diff
            if (diff .gt. eps) num = num + 1
```

3.3 Scalar versus Vectors

1. Huge disparity in performance (scalar / vector).
2. Programs, algorithms, database design more closely related to the architecture.
3. More sensitivity to compiler efficiency.

A *vector operation* is a hardware instruction in which source and result operands are streams of data *(vectors)*. Pipelining and separating the functional unit helps. A *vectorizable computation* is one that can be carried out *efficiently* with vector operations. A *vector* is a collection of data which qualify as operands in a vector operation (instruction). In the Cyber 205, data is stored contiguously in memory. In the Cray-2, a collection with stride that is not a multiple of 128 is a vector. See Figures 3.5 and 3.6.

On the EDSAC-1 in 1949, a minor cycle equals $2\mu s$ or $2 \times 10^3 n$ seconds. The peak speed equals 100 ops / sec. On the Cray-2, $\tau = 4.1$ nsec and $r_\infty = 400$ mflops. $\frac{2000 \text{ nsecs}}{4.1} = 500-$fold increase in speed. $\frac{400 \times 10^6}{100} = 4 \times 10^6$ increase in peak performance due to architecture built by designers.

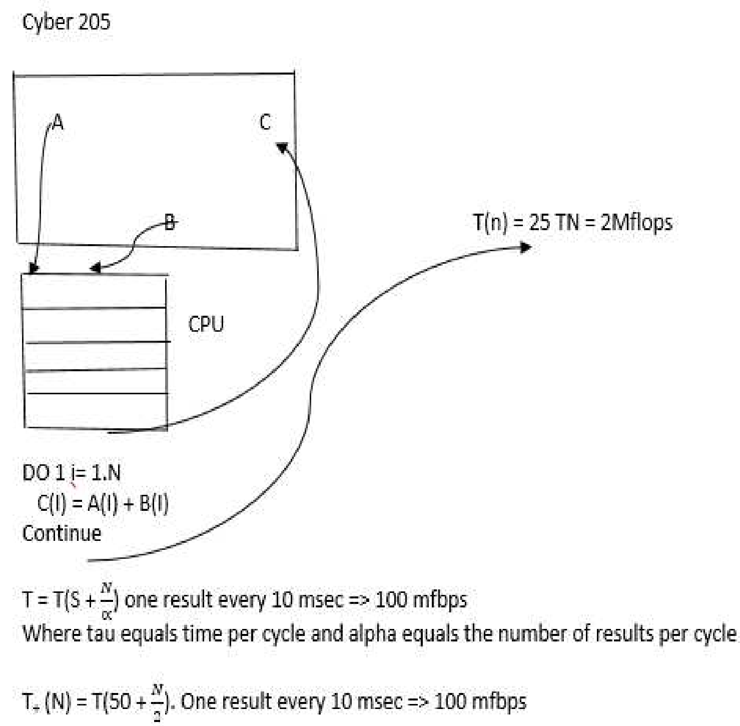


Figure 3.5: This figure shows the Cyber 205

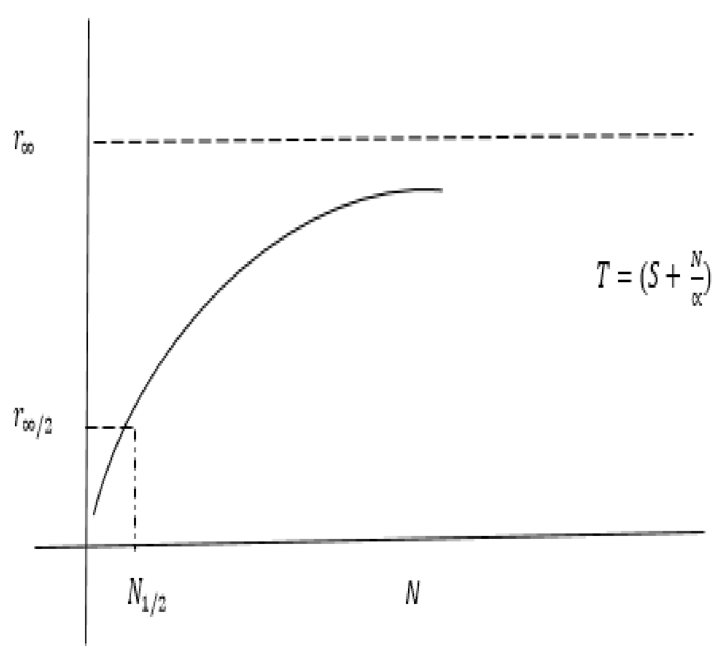


Figure 3.6: This figure shows a graph of N versus r.

- Overlap:
  1. Broad scale
     (a) Overlap CPU and I/O activity
     (b) Multiprogramming
     (c) Independent functional units
  2. Finer scale
     (a) Pipelining — CPU, memory fetch process, instruction decoding
- Replication:
  1. Multiple functional units (pipelines)
  2. Multiple CPU's

History of Parallelism in Computing

1949 EDSAC — University of Cambridge. First stored program computer. Bit serial. Took 32 cycles to add two 32-bit quantities.

1952 IBM 701 — First parallel arithmetic — electrostatic cathode ray tube storage.

1955 IBM 704 — First magnetic core memory. First floating point hardware.

1955 IBM 709 — Re-engineered 704 with I/O channel. Worked independent of CPU.

1962 ATLAS — University of Manchester. Complex operating system including multiprogramming and virtual memory. Had banked memory and multiple functional units.

1964 CDC 6600 — Seymour Cray. Lots of parallelism. Ten functional units. Ten peripheral processors (early example of parallel processing). Thirty two banks of memory. Look-ahead instruction fetch and decode. Significant market impact.

Vector Computers:

1964 CDC STAR-100 computer — 100 Mflops for long vectors, but slow scalar, short vector, and non-unit stride. Only three made. Virtual memory (0.5 Mwd) 40 nsec cycle. Multiple pipes (Langley received 2-pipe machine in 1977). Memory to memory.

1980 CYBER-203 — Electronic memory (1Mwd). Separate scalar unit increased scalar speed by six and improved non-unit stride.

1984 CYBER-205 — Halved minor cycle speed. Increased speed by 4 on some instructions and introduced linked triad that could achieve 800 Mflops. Reduced startup times.

1976 CRAY-1 — Register to register. 12.5 nsec cycle. Single load / store. Pipe a negative. Better vectoring software than CDC.

1980 CRAY-XMP — Redesigned CRAY-1 (Steve Chen). Multiple ports. Automatic chaining. Multiple CPU's. 8.5 nsec cycle.

1985 CRAY-2 — Huge memory gain compared to the CRAY-1 (256Mwds but slow). 4.1 nsec cycle.

1989 CRAY-YMP — Faster than the CRAY-XMP (6 Nsec). Up to 8 CPU's and 128 Mwds.

1992 CRAY C-90 — Up to 16 processors. 4 clocks. 4 results / clock.

Parallel Computers:

1970 Illiac IV

1988 Intel IPSC/860 — CRAY on a chip. MIMD CM-2. 65,000 1-bit processors. SIMD.

1992 Intel Paragon — Mesh routing. 25% faster chip. CM-5. Full processors. SIMD and MIMD capability. Vector units. Kendall square. Shared memory paradigm.

1993 CRAY, Convex, et al.

3.3.1 Linear Algebra

Compute $\bar{b} = A\bar{x}$ where matrix A is an $n \times n$ matrix and $\bar{b}, \bar{x}$ are $n \times 1$ vectors.

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ a_{21} & \cdots & \cdots & \cdots & a_{2n} \\ \vdots & & & & \vdots \\ a_{n1} & \cdots & \cdots & \cdots & a_{nn} \end{bmatrix}, \quad \bar{X} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad \bar{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}.$$

a_{ij} resides in the i^{th} row of the j^{th} column in matrix A. The inner-product (also called the dot product) of vectors $\bar{a}$ and $\bar{b}$ is defined as $< \bar{a}, \bar{b} >= a_1b_1 + a_2b_2 + \cdots + a_nb_n = \sum_{j=1}^{n} a_jb_j$. The notation $b = Ax$ means

$$b_i = \sum_{j=1}^{n} a_{ij}X_j = < i^{th} \text{ row of } A, \ \bar{x} > .$$

Example: Let $n = 3$. Then, for the equations $b = Ax$,

$$\begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \end{bmatrix} \begin{bmatrix} x_1 \\ x_1 \\ x_1 \end{bmatrix} + \begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \end{bmatrix} \begin{bmatrix} x_2 \\ x_2 \\ x_2 \end{bmatrix} + \begin{bmatrix} a_{13} \\ a_{23} \\ a_{33} \end{bmatrix} \begin{bmatrix} x_3 \\ x_3 \\ x_3 \end{bmatrix}$$

is the inner-product formation. The outer-product uses vector multiplication and vector addition. See Figure 3.7.

For the system of equations $Ax = b$, solve for $\bar{x}$. The solution is $x = A^{-1}b$. We can factor $A = LU$ which is called *LU factorization* where

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ l_{21} & 1 & 0 & 0 & \cdots & 0 \\ l_{31} & l_{32} & 1 & 0 & \cdots & 0 \\ \cdots & \cdots & & & \vdots & \cdots \\ l_{n1} & l_{n2} & l_{n3} & \cdots & \cdots & 1 \end{bmatrix}, \quad U = \begin{bmatrix} u_{11} & u_{12} & \cdots & \cdots & u_{1n} \\ & u_{22} & \cdots & \cdots & u_{2n} \\ \cdots & \cdots & u_{32} & \vdots & u_{2n} \\ & & & & u_{nn} \end{bmatrix}.$$

$LUx = b$. $L(Ux) = b$. $Ly = b$ where $y = Ux$. The forward solve is $y_1 = b_1$. $l_{21}y_1 + y_2 = b_2 \Rightarrow y_2 = b_2 - l_{21}y_1$. $l_{31}y_1 + l_{32}y_2 + y_3 = b_3 \Rightarrow y_3 = b_3 - l_{32}y_2 - l_{31}y_1$. The back-solve is $x_3 = \frac{y_3}{u_{33}}$. $x_2 = \frac{y_2 - u_{23}x_3}{u_{22}}$. It takes $\bigcirc(\frac{2}{3}n^3)$ to compute L and U. Therefore, for the forward solve $\bigcirc(n^2)$ and for the back-solve $\bigcirc(n^2)$. To compute the inverse of the matrix $\bigcirc(2n^3) \to \bigcirc(2n^2)$.

A tridiagonal matrix looks like:

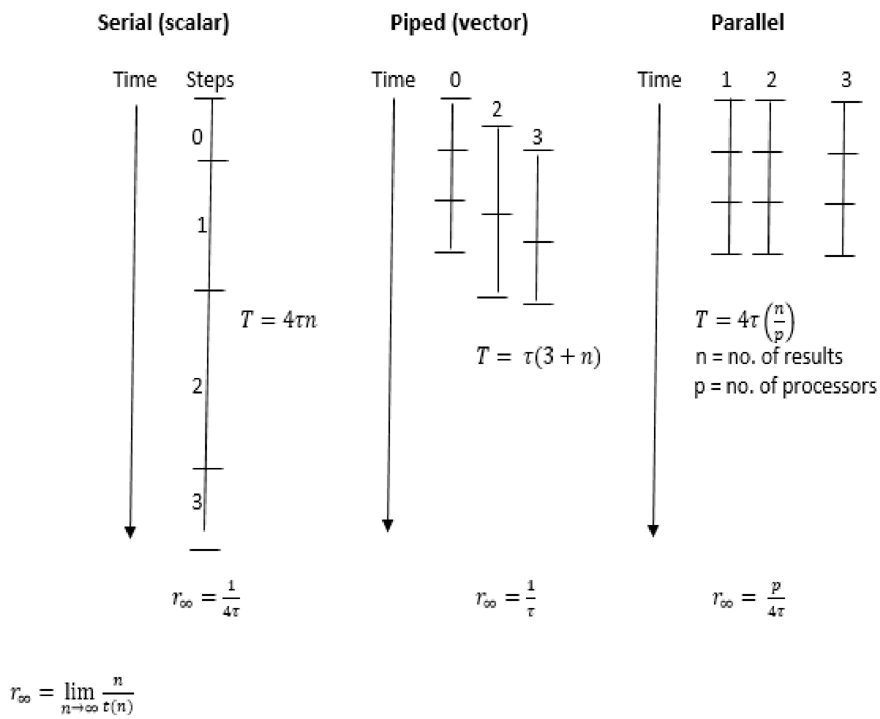


Figure 3.7: This figure shows a diagram of the timing of serial, piped, and parallel computers.

$$
\begin{bmatrix}
x & x & & & & & & & \\
x & x & x & & & & 0 & & \\
 & x & x & x & & & & & \\
 & & x & x & x & & & & \\
 & & & x & x & x & & & \\
 & & & \ddots & \ddots & \ddots & & & \\
 & & & & x & x & x & & \\
 & & 0 & & & x & x & x & \\
 & & & & & & & x & x
\end{bmatrix}
=
\begin{bmatrix}
1 & & & & & & & \\
x & 1 & & & & 0 & & \\
 & x & 1 & & & & & \\
 & & x & 1 & & & & \\
 & & & x & 1 & & & \\
 & & & & x & 1 & & \\
 & & & & \ddots & \ddots & & \\
 & & 0 & & & x & 1 & \\
 & & & & & & x & 1
\end{bmatrix}
\begin{bmatrix}
x & & & & & & & \\
x & x & & & & 0 & & \\
 & x & x & & & & & \\
 & & x & x & & & & \\
 & & & x & x & & & \\
 & & & & x & x & & \\
 & & & & \ddots & \ddots & & \\
 & & 0 & & & x & x & \\
 & & & & & & x & x
\end{bmatrix}.
$$

Decomposition proof. Let

$$
A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = A^{(1)}.
$$

$l_{ij} = \frac{a_{ij}}{a_{ji}}$ form:

1. $l_{21} = \frac{a_{21}}{a_{11}}$. Replace row 2 by row 2 minus l_{21} times row 1.
2. $l_{31} = \frac{a_{31}}{a_{11}}$. Replace row 3 by row 3 minus l_{31} times row 1.

$$
A^{(2)} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} \\ 0 & a_{32}^{(2)} & a_{33}^{(2)} \end{bmatrix}
$$

3. $l_{32} = \frac{a_{32}^{(2)}}{a_{33}}$. Replace row 3 by row 3 minus l_{32} times row 2.

$$A^{(3)} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} \\ 0 & 0 & a_{33}^{(3)} \end{bmatrix} = U.$$

$$L = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix}.$$

We wish to do the following:

(a) Multiply a row of matrix A by a scalar (scale row).
(b) Replace a row of matrix A by itself minus another scaled row.

Then,

(a) Performing the above operations on the unit matrix.
(b) Pre-multiplying matrix A by that matrix.

Example: Let matrix A be

$$A = \begin{bmatrix} 1 & 2 & 1 \\ 4 & 1 & 2 \\ 2 & 0 & 3 \end{bmatrix}$$

Compute row 3 $\leftarrow$ row 3 $-2*$ row 1. $(0\ \ -4\ \ 1) \leftarrow (2\ \ 0\ \ 3) - 2(1\ \ 2\ \ 1)$.

$$I_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -2 & 0 & 1 \end{bmatrix} = I_3'.$$

Then,

$$I_3'A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -2 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 1 \\ 4 & 1 & 2 \\ 2 & 0 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 1 \\ 4 & 1 & 2 \\ 0 & -4 & 1 \end{bmatrix}.$$

Define

$$L_{21} = \begin{bmatrix} 1 & 0 & 0 \\ -l_{21} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad L_{31} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -l_{31} & 0 & 1 \end{bmatrix}.$$

$$L_{31}(L_{21}A) \rightarrow \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22}^{(2)} & a_{23}^{(2)} \\ 0 & a_{32}^{(2)} & a_{33}^{(2)} \end{bmatrix},$$

$$L_{31}(L_{21}) = \begin{bmatrix} 1 & 0 & 0 \\ -l_{21} & 1 & 0 \\ -l_{31} & 0 & 1 \end{bmatrix} = L_1.$$

$$L_{32} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -l_{32} & 1 \end{bmatrix} = L_2.$$

$L_2 L_1 A = U$. $A = L_1^{-1} L_2^{-1} U$. If

$$L_1 = \begin{bmatrix} 1 & 0 & 0 \\ -l_{21} & 1 & 0 \\ -l_{31} & 0 & 1 \end{bmatrix}$$

Then, the inverse of L_1 is

$$L_1^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & 0 & 1 \end{bmatrix}.$$

$$L_1^{-1} L_2^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix}.$$

Therefore, $A = LU$.

3.3.2 Decomposition

Decomposition of matrix A where $Ax = b$ and $A = LU$. The forward solve is $Ly = b$. The back-solve is $Ux = y$.

1. Forward solve.
2. Do forward solve with decomposition.

$$\begin{aligned} &Ax = b, \\ &L_1 A \to A^{(2)},\ \ L_1 A x = L_1 b, \\ &L_2 A^{(2)} x = L_2 (L_1 b), \\ &Ux = b''. \end{aligned}$$

No extra storage is needed. Place the $l'_{ij}s$ in the lower part of the new matrix.

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ l_{21} & a_{22} - l_{21}a_{12} & a_{23} - l_{21}a_{13} & a_{24} - l_{21}a_{14} \\ l_{31} & a_{32} - l_{31}a_{12} & a_{33} - l_{31}a_{13} & a_{34} - l_{31}a_{14} \\ l_{41} & a_{42} - l_{41}a_{12} & a_{43} - l_{41}a_{13} & a_{44} - l_{41}a_{14} \end{bmatrix}$$

We can define one vector as

$$\begin{bmatrix} l_{21} \\ l_{31} \\ l_{41} \end{bmatrix} = \begin{bmatrix} a_{21} \\ a_{31} \\ a_{41} \end{bmatrix}.$$

$n-1$ vector subtractions and $n-1$ vector multiplications are needed. Pivot the row with the largest number in a column. The vector syntax for the Cyber-205 is A(FWA, LT) where FWA means first word address, A(FWA) is a vector name, and LT is the length of the vector. For example, $A(1,1;4)$ is the first column of matrix A.

$$A = \begin{bmatrix} 1,1 & 1,2 & 1,3 & 1,4 \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \downarrow & \downarrow & \downarrow & \downarrow \\ 4,1 & 4,2 & 4,3 & 4,4 \end{bmatrix}.$$

$A(1,2;8)$ is the middle two columns or $k := 2$, $N = 4$, $A(1,k;2*N)$. Look at the forward solve $Ly = b$.

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ l_{21} & 1 & 0 & 0 \\ l_{31} & l_{32} & 1 & 0 \\ l_{41} & l_{42} & l_{43} & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}.$$

1. Without storing solutions in $\bar{b}$ but in $\bar{y}$:

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 - l_{21}y_1 \\ b_3 - l_{31}y_1 - l_{32}y_2 \\ b_4 - l_{41}y_1 - l_{42}y_2 - l_{43}y_3 \end{bmatrix}$$

2. Scalar codes:

```
1 [ DO 2 i = 2, N-1
  [ S = B(i)
  [ 2 [ DO 1 j = 1, i-1
  [   [ 1 S = S - A(i,j) * B(j)
  [ C S is now y(i)
  [ 2 B(i) = S
```

3. Vector code:

```
1 [ DO 1 i = 2, N
  [ [ LT = N - j + 1
  [ [ B(i; LT) = B(i; LT) - A(i,i-1; LT) * B(i-1)
  [ 1 Continue
```

3.3.3 Homework

Let

$$A = \begin{bmatrix} 6 & 3 & -3 & 6 \\ 2 & 7 & 2 & 5 \\ 2 & 4 & 5 & 1 \\ -4 & 4 & 1 & -1 \end{bmatrix}, \quad b = \begin{bmatrix} 0 \\ -3 \\ 3 \\ 7 \end{bmatrix}.$$

What are L, U, and x? Write $Ux = y$ code in three steps mentioned in class for the back-solve. Write the code for Gaussian elimination (no three steps involved) decomposition methods.

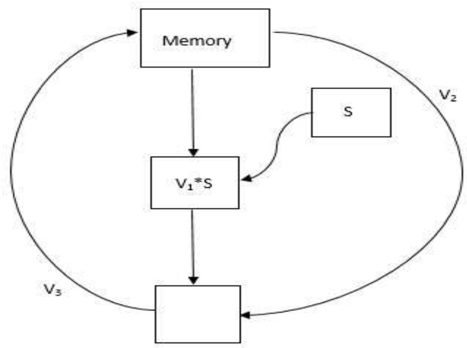


Figure 3.8: This figure shows storing results in memory for the linked triad example.

3.4 Cyber 205

Memory:

- 32 mwds (64 bit).
- Virtual memory.
- Small page — 512 wds.
- Large page — 65K words (128 sm pgs).

The virtual memory never worked as they would like. The virtual memory is bit addressable. It has super-word access (8×64 bits) = super-word = 512. Some comments on the CPU speed:

- Memory to memory vectors.
- Vector $\Leftrightarrow$ consecutive locations.
- Register to register scalars (256 scalar registers).
- 20 nanosec cycle time (τ). $\frac{1}{\tau} = 50$ million cycles / second.
- 1, 2 or 4 pipes each returning one result per cycle with the exception of linked triad. See Figure 3.8. The following equations give an example of linked triads.

$$
\begin{aligned}
&V_3 = V_1 + S * V_2 \\
&V_3 = S + V_1 * V_2 \\
&V_3 = S * (V_1 + V_2)
\end{aligned}
$$

Example: An example of a linked triad. 4 pipes $\rightarrow$ 200 mflops. 32 bit $\rightarrow 200 \times 2$. Linked triad $\rightarrow 200 \times 2$. Therefore, 800 mflops is the peak speed.

Example: Assume 11 functional units. $\tau = 20$ nsecs. One result each, 10 nsecs $\rightarrow$ 100 mflops. Must get 4 operands to the CPU or 1 operand per 5 nsecs $\Rightarrow$ bandwidth 200 mwds / sec. One result per 10 nsecs $\Rightarrow$ 100 mwrd / sec. A super-word has 512 bits = 8 words / cycle or 1 word / 2.5 nsec = 400 mwds / sec $\Rightarrow$ bandwidth is sufficient to support the computation.

```
                        A(1)         A(2)   ......      A(8)
32 banks   \             |            |                   |
            512          |            |                   |
16 stacks  /             |            |                   |
                         |            |                   |
                       Stack        Stack               Stack
```

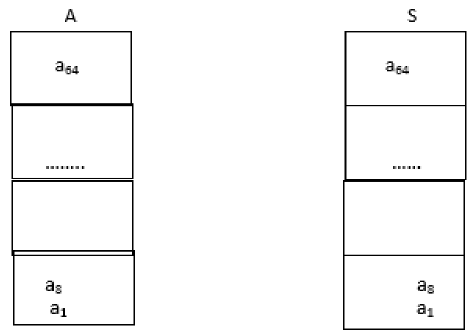


Figure 3.9: This figure shows the memory for approximating division on a Cray.

On the Crays, estimates of division are used. The Newton iteration is performed.

$$f(x+h) = f(x) + hf'(x) + \bigcirc(h^2) = f(x) + hf'(x).$$

Choose h such that $x_1 = x + h$ satisfies $f(x_1) = 0$. So, $0 = f(x_1) = f(x) + (x_1 - x)f'(x)$, $x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$. Suppose $f(x) = b - \frac{1}{x}$. $f(x_1) = 0 = b - \frac{1}{x_1}$. $x_i = \frac{1}{b}$. $f'(x) = \frac{1}{x^2}$.

$$x_1 = x_0 - \frac{(b - \frac{1}{x_0})}{\frac{1}{x_0^2}} = x_0 - bx_0^2 + x_0 = x_0(2 - bx_0).$$

To compute a/b :

1. Get an approximation to $1/b(x_0)$.

2. $v_1 = 2 - b * x_0$.

3. $v_2 = v_1 * x_0$ ($x_1 = 1/b$ to $\sim$ 48 bits).

4. $v_3 = a * v_2$.

Example: Find $\sqrt{b}$. Solution: $f(x) = b - \frac{1}{x^2}$. $f(x_1) = 0 \Rightarrow x_1 = \frac{1}{\sqrt{b}}$. Assume $x_0 = \frac{1}{\sqrt{b}}$. $f'(x) = \frac{2}{x^3}$.

$$x_1 = x_0 - \frac{b - \frac{1}{x_0^2}}{\frac{2}{x_0^3}} = \frac{3}{2}x_0 - \frac{x^3 b}{2}$$

where the last two terms are approximations provided by the Cray-2.

Compute $\sum_{i=1}^{64} a_i$. See Figure 3.9. $A(i+8) + S(i) \rightarrow S_{i+8}$, $i = 1, 56, ...$

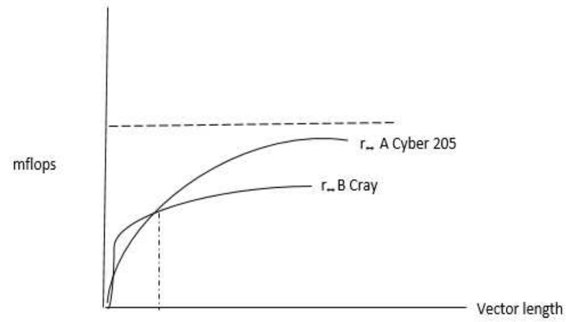


Figure 3.10: This figure shows a comparison of two machines A and B.

$$
\begin{aligned}
&a_9 + S_1 \to S_9, \;\; (a_9 + a_1)\\
&a_{10} + S_2 \to S_{10}, \;\; (a_{10} + a_2)\\
&\vdots\\
&a_{16} + S_8 \to S_{16}, \;\; (a_{16} + a_8)\\
&a_{17} + S_9 \to S_{17}, \;\; (a_{17} + a_9 + a_1)\\
&\vdots\\
&a_{24} + S_{16} \to S_{24}, \;\; (a_{24} + a_{16} + a_8)\\
&a_{25} + S_{17} \to S_{25}, \;\; (a_{25} + a_{17} + a_9 + a_1)\\
&\vdots\\
&S_{57} = a_{57} + a_{49} + a_{41} + \cdots + a_1\\
&S_{58} = a_{58} + \cdots + a_2\\
&\vdots\\
&S_{64} = a_{64} + a_{56} + \cdots + a_8
\end{aligned}
$$

Therefore, the problem is reduced to summing eight numbers S_{57} to S_{64}.

3.4.1 Performance Analysis

The computing rate is $r(n) = \dfrac{\text{mflops}}{\text{sec}}$ = number of floating-point operations divided by time. If $f(n)$ defines the number of operations, then $r(n) = \frac{f(n)}{t(n)}$. $r_\infty = \lim_{n\to\infty} r(n) = \lim_{n\to\infty} \frac{f(n)}{t(n)}$ tells how fast the machine can go (under the best circumstances is assumed). $n_{\frac{1}{2}}$ = vector length at which the machine achieves $\frac{1}{2}$ of r_∞.

Consider Figure 3.10. Which machine is better, A or B? We would want machine A if large vector lengths are going to be used. We would want machine B if short vector lengths are anticipated.

3.4.2 Linked Triad Example on the Cyber 205

$T(n) = \tau\left(83 + \frac{n}{2}\right)$, $\tau = 20 \times 10^{-9}$ sec. $f(n) = 2n$

$$r(n) = \frac{2n \times 10^{-6}}{20 \times 10^{-9}(83 + \frac{n}{2})} = \frac{200n}{166 + n}.$$

$$\lim_{n\to\infty} r(n) = \lim_{n\to\infty} \frac{200n}{166 + n} = \frac{200}{0 + 1} = 200.$$

Solve for $n_{\frac{1}{2}}$.

$$\frac{200n}{166+n} = 100,$$

$$200n = 16600 + 100n,$$

$$n_{\frac{1}{2}} = 166.$$

The vector length must be at least 166.

Suppose $F(n) = mn$ for vector length n. $T(n) = \tau(S + \alpha(mn)) = \tau\alpha m(C+n)$, where $C = \frac{S}{\alpha m}$. $r(n) = \frac{F(n)}{T(n)} = \frac{mn}{\tau\alpha m(C+n)} = \frac{n}{T\alpha(C+n)}$. $\lim_{n\to\infty} \frac{n}{T\alpha(C+n)} = \frac{1}{\tau\alpha}$. α is a constant that is a function of the hardware used. $\frac{\widehat{n}}{\tau\alpha(C+\widehat{n})} = \frac{1}{2\tau\alpha}$, where $\widehat{n} = \frac{C+\widehat{n}}{2} \Rightarrow \widehat{n} = C$.

Example: $f(n) = 2n \Rightarrow m = 2$. $T(n) = \tau(83 + \frac{n}{2}) = \frac{\tau}{2}(166+n) = \frac{2\tau}{4}(166+n)$. Therefore, $\alpha = \frac{1}{2}$. $r_\infty = \frac{1}{\alpha T} = \frac{T^{-1}}{\alpha} = 4\tau^{-1}$.

Example: For the Cyber 205, $\tau = 20$ nsec and $T^{-1} = 50$ mflops.

Example: For the Cray, $\tau = 6$ nsec and $T^{-1} = 166$ mflops.

Example: For the Star, $\tau = 60$ nsec and $T^{-1} = 25$ mflops.

Example: For the vector divide problem on the Cyber 205, let $T(n) = \tau\left(80 + \frac{n}{0.25}\right)$. $f(n) = n = (1)(n) \Rightarrow m = 1$. $\tau(80+4n) = 4\tau(20+n) \Rightarrow n_{\frac{1}{2}} = 20 \Rightarrow r_\infty = \frac{\tau^{-1}}{\alpha} = \frac{50}{4} = 12.5$

Example: For the inner-product problem on the Cyber 205, where vector one is gathered from a row of an array, the procedure is to:

1. Gather data of length n.
2. Calculate the inner-product.

Step 1 takes $T = \tau\left(39 + \frac{n}{0.8}\right)$ amount of time. Step 2 takes $T = \tau(116+n)$ amount of time. $f(n) = 2n \Rightarrow m = 2$.

$$T(n) = \tau\left(39 + \frac{5}{4}n + 116 + n\right) = \tau(115 + \frac{9}{4}n) = \frac{9}{4}\tau\left(\frac{155}{9/4} + n\right) \Rightarrow$$

$$C = n_{\frac{1}{2}} = \frac{4(155)}{9} = 69,$$

$$\frac{9}{8}(2)\tau\left(\frac{155}{9/4} + n\right)$$

where $\alpha = \frac{9}{8}$, $m = 2$, and $C = 69$.

$$r_\infty = \left(\frac{8}{9}\right)50 = 44 \text{ mflops}.$$

Average Vector Lengths

Theorem: A series of k similar vector operations, whose average vector length is $\bar{n}$, has the same performance as if all k vector operations were of length $\bar{n}$. Prove that $T = \tau k\left(S + \frac{k}{L}\right)$. Proof:

$$T = \tau \sum_{i=1}^{k} S + \frac{n_i}{L} = TkS + \frac{\tau}{L}\sum_{i=1}^{k} n_i = \tau k\left(S + \frac{k}{L}\sum_{i=1}^{k}\frac{n_i}{k}\right) = \tau k\left(S + \frac{\bar{n}}{L}\right).$$

Identities

1. $\sum_{k=1}^{n} k = \frac{n(n+1)}{2}$.

2. $\sum_{k=1}^{n} \alpha = n\alpha$.

3. $\sum_{k=1}^{n} k^2 = \frac{n(n+1)(2n+1)}{6}$.

Determine the average vector length $\bar{n}$ in Gaussian elimination. The average vector length is

$$\frac{\sum \text{ vector lengths}}{\sum \text{ vector instructions}} = \bar{n}.$$

$$1\left[\begin{array}{l}\textbf{FOR } \mathrm{j = 1, n\text{-}1} \\ 2\left[\begin{array}{l}\textbf{FOR } \mathrm{i = j+1, n} \\ L_{ij} = a_{ij}/a_{ii} \to a_{ij}\end{array}\right.\end{array}\right.$$

$$1\left[\begin{array}{l}\textbf{FOR } \mathrm{k = j+1, n} \text{ (modify column k)} \\ 2\left[\begin{array}{l}\textbf{FOR } \mathrm{i = j+1, n} \\ a_{ik} = a_{ik} - L_{ij} * a_{jk} \text{ (linked triad)}\end{array}\right.\end{array}\right.$$

At the j^{th} step, have $n - j$ linked triads of length $n - j$.

$$\bar{n} = \frac{\sum_{j=1}^{n}(n-j)(n-j)}{\sum_{j=1}^{n-1}(n-j)} = \frac{\sum_{j=1}^{n}(n^2 - 2nj + j^2)}{\sum_{j=1}^{n-1}(n-j)} = \frac{n^3 - \frac{2n(n)(n+1)}{2} + \frac{n(n+1)(2n+1)}{6}}{n(n-1) - \frac{n(n-1)}{2}} = \frac{\bigcirc\frac{n^3}{3}}{\bigcirc\frac{n^2}{2}} = \bigcirc\left(\frac{2}{3}n\right).$$

Example: Suppose $f(n) = mn$. $T(n) = \tau(S + \alpha mn) = \alpha m\tau(C + n)$ where $C = \frac{S}{\alpha m}$. $r_\infty = \frac{1}{\tau\alpha}$. $n_{\frac{1}{2}} = C$. $\tau = 4.1$ nsec for the Cray-2. $\tau = 6$ nsec for the Cray-YMP.

Example: Suppose the operation count is $F(n) = f(n)\bar{n}$. $T(n) = \tau(S + \alpha f(n)\bar{n}) = \alpha f(n)\tau(C + \bar{n})$. $r_\infty = \frac{1}{\tau\alpha}$. $n_{\frac{1}{2}} = C$. $n_{\frac{1}{2}}$ is the value of $\bar{n}$ which you get $\frac{1}{2}$ of r_∞. $r_\infty = \frac{1}{\tau\alpha}$.

Example: Suppose we have n vector adds each of length n on a two pipe Cyber-205. $F(n) = n^2$. $\bar{n} = n$. $f(n) = n$. Suppose $T_4 = \tau\left(50 + \frac{n}{2}\right)$. $T = n\tau\left(50 + \frac{n}{2}\right) = \frac{n}{2}\tau(100 + n) = n\left(\frac{1}{2}\right)\tau(100 + n)$. $\alpha = \frac{1}{2}$. Then, $r_\infty = \frac{1}{\tau\alpha} = \frac{2}{\tau} = 100$ mflops. $n_{\frac{1}{2}} = 100$.

Example: $2n^2$ flops using $4n$ vector adds of one length $\frac{n}{2}$. What is r_∞? And for what problem size n do we get half performance? $F(n) = 2n^2 = (4n)\frac{n}{2}$. $T(n) = 4n\tau(50 + \frac{\bar{n}}{2}) = 2n\tau(100 + \bar{n}) = (4n)\frac{1}{2}\tau(100 + \bar{n})$. $\bar{n}_{\frac{1}{2}} = 100$. $r_\infty = \frac{2}{\tau} = 100$. The problem size should be $n = 200$.

3.4.3 Homework

Use 64-bit numbers.

1. Inner-product on Star-100, $T = \tau(100 + 4n)$, $\tau = 40$ nsecs. Solution: The inner-product on the Star-100, $T(n) = \tau(100 + 4n)$, $\tau = 40$ nsec. $F(n) = 2n$. $T(n) = 4\tau(25 + n) = 2(4)\tau(25 + n) \Rightarrow n_{\frac{1}{2}} = 25 \Rightarrow r_\infty = \left(\frac{1}{\tau}\right)\left(\frac{1}{2}\right) = 12.5$ mflops.
2. Vector sum on Cyber-205. Solution: $F(n) = n$. $T(n) = \tau(116 + n) = 1(1)\tau(116 + n) \Rightarrow n_{\frac{1}{2}} = 116 \Rightarrow r_\infty = 50$ mflops.
3. Two vector adds and one vector divide on a 4-pipe Cyber-205. $\tau\left(S + \frac{n}{4}\right)$. Solution: $F(n) = 3n$. $T(n) = \tau[2(51 + \frac{n}{4}) + 80 + \frac{n}{0.56}] = \tau(182 + 2.28n) = 2.28\tau(79.6 + n)$. $T(n) = 3\left(\frac{2.28}{3}\right)\tau(79.6 + n) \Rightarrow r_\infty = \frac{1}{\tau\alpha} = \left(\frac{3}{2.28}\right)(50) = 68 \Rightarrow n_{\frac{1}{2}} = 79.6$. $\alpha = 3$.

3.4.4 Homework

For a 4-pipe Cyber-205, $2n$ vector multiplies and inner-product of average length $\frac{2}{3}n$. Find f_∞ and the value of n that we get $\frac{1}{2}r_\infty$.

3.5 Cray Timing

	Cray-2	Cray-YMP
Load / Store	$34 + L$	$19 + L$
Add	$22 + L$	$11 + L$
Multiply	$22 + L$	$12 + L$

where $L \leq 64$. $T(L) = \tau(S + \alpha mL)$, $L \leq 64$, $n = \beta L \Rightarrow \beta = \frac{n}{L}$. $T(n) = \tau[LSU + \beta(S + \alpha mL)] = \tau[LSU + \frac{n}{64}(S + \alpha m(64))] = \tau[LSU + n(\frac{S}{64} + \alpha m)]$.

Example: Consider a symmetric matrix where the elements $a_{ij} = a_{ji}$. Devise a stride one algorithm which only uses one-half the matrix.

$$\begin{bmatrix} a_{11} & a_{21} & a_{31} & a_{41} & a_{51} \\ a_{21} & a_{22} & a_{32} & a_{42} & a_{52} \\ a_{31} & a_{32} & a_{33} & a_{13} & a_{53} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{54} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} \rightarrow \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix}$$

Solutions:

1. $b_1 = b_1 + < (a_{21},\ a_{31},\ a_{41},\ , a_{51}), (x_2,\ x_3,\ x_4,\ x_5) >$.

$$\begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \\ a_{41} \\ a_{51} \end{bmatrix} x_1.$$

2. $b_2 = b_2 + < (a_{32},\ a_{42},\ , a_{52}), (x_3,\ x_4,\ x_5) >$.

$$\begin{bmatrix} b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix} = \begin{bmatrix} b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix} + \begin{bmatrix} a_{22} \\ a_{32} \\ a_{42} \\ a_{52} \end{bmatrix} x_2.$$

We want to solve $Ax = R$.

$$\begin{bmatrix} a_1 & b_1 & & & \\ c_2 & a_2 & b_2 & & \\ & c_3 & a_3 & b_3 & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots \end{bmatrix} = \begin{bmatrix} 1 & & & & & \\ L_2 & 1 & & & & \\ & L_3 & 1 & & & \\ & & L_4 & 1 & & \\ & & & \ddots & \ddots & \\ & & & \ddots & \ddots & \\ & & & & L_n & 1 \end{bmatrix} \begin{bmatrix} u_1 & b_1 & & & & \\ & u_2 & b_2 & & & \\ & & u_3 & b_3 & & \\ & & & u_4 & b_4 & \\ & & & \ddots & \ddots & \\ & & & \ddots & \ddots & \\ & & & & u_n & b_n \end{bmatrix}$$

Solve $Ly = R$ with forward substitution. Solve $Ux = y$ with backward substitution. We can use the following factorization algorithm (Thomas' algorithm): define $d_i = \frac{1}{u_i}$. $d_1 = \frac{1}{a_1}$. $L_i = c_i d_{i-1}$. $d_i = \frac{1}{a_i - L_i b_{i-1}}$ where $i = 2, 3, ..., n$. The forward solve for $Ly = R$ is $y_1 = R_1$, $y_i = R_i - L_i y_{i-1}$, $i = 2, ..., n$. The back solve is $x_n = y_n d_n$, $x_i = (y_i - x_{i+1} b_i) d_i$, $i = n-1, n-2, ..., 1$. The algorithm is on the order $\bigcirc(n)$. Thomas' algorithm is all recursive.

Stone's recursive doubling algorithm is as follow. Given $a_1, a_2, ..., a_n$, compute $p_j = \prod_{k=1}^{\gamma} a_k$.

$$\begin{aligned} &p_1 = a_1 \\ &p_2 = a_1 a_2 \\ &\vdots \\ &p_n = a_1 a_2 \cdots a_n \end{aligned}$$

The serial algorithm is

$P(1) = n(n)$.
For $j = 2, n$ $P(j) = P(j-1)A(j)$

So, define $s_{ij} = \prod_{k=i}^{\gamma} a_k$.

$$\begin{aligned} &s_{1j} = P_j \\ &s_{ij} s_{j-1,k} = s_{i,k} \end{aligned}$$

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_n \end{bmatrix} \begin{bmatrix} --- \\ a_1 \\ a_2 \\ \vdots \\ a_{n-1} \end{bmatrix} = \begin{bmatrix} a_1 \\ a_1 a_2 \\ a_2 a_3 \\ \vdots \\ a_{n-1} a_n \end{bmatrix} = \begin{bmatrix} s_{11} \\ s_{12} \\ s_{23} \\ \vdots \\ \vdots \\ \vdots \\ s_{n-1} s_n \end{bmatrix} \begin{bmatrix} --- \\ --- \\ s_{11} \\ s_{12} \\ s_{23} \\ \vdots \\ s_{n-3} s_{n-2} \end{bmatrix} = \begin{bmatrix} s_{11} \\ s_{12} \\ s_{13} \\ s_{14} \\ s_{25} \\ \vdots \\ s_{n-3} s_n \end{bmatrix}.$$

Assume $n = 8$. Then,

$$\begin{bmatrix} s_{11} \\ s_{12} \\ s_{13} \\ s_{14} \\ s_{25} \\ s_{36} \\ s_{47} \\ s_{58} \end{bmatrix} \begin{bmatrix} --- \\ --- \\ --- \\ --- \\ s_{11} \\ s_{12} \\ s_{13} \\ s_{14} \end{bmatrix} = \begin{bmatrix} s_{11} \\ s_{12} \\ s_{13} \\ s_{14} \\ s_{15} \\ s_{16} \\ s_{17} \\ s_{18} \end{bmatrix}.$$

Let's try to cast the tridiagonal solution in the above way. $y_1 = r_1$, $y_i = r_i - L_i y_{i-1}$, $L = 2, 3, ..., n$. Define

$$y_i = \begin{bmatrix} y_i \\ 1 \end{bmatrix}.$$

$$y_i = \begin{bmatrix} y_i \\ 1 \end{bmatrix} = \begin{bmatrix} -L_i & r_i \\ 0 & 1 \end{bmatrix} \begin{bmatrix} y_{i-1} \\ 1 \end{bmatrix} = H_i y_{i-1}.$$

$$y_i = \left(\prod_{j=2}^{i} H_j \right) y_1 = H_{2,i} y_1.$$

$$\begin{bmatrix} H_2 \\ H_3 \\ H_4 \\ \vdots \\ H_8 \end{bmatrix} \begin{bmatrix} --- \\ H_2 \\ H_3 \\ \vdots \\ H_7 \end{bmatrix} = \begin{bmatrix} H_2 \\ H_{23} \\ H_{34} \\ \vdots \\ H_{78} \end{bmatrix} \begin{bmatrix} --- \\ --- \\ H_2 \\ \vdots \\ H_{67} \end{bmatrix}.$$

Consistent Vectorization

A vectorization that requires the same order of magnitude of operations as the best serial algorithm it replaces is called a *consistent vectorization.* $\log_2 n$ at the k^{th} step, the vector length equal to $n - 2^{k-1}$,

$$\sum_{k=1}^{\log_2 n} 2^{k-1} = n - 1 = \sum_{k=1}^{\log n} \frac{n}{2^k}.$$

The average vector length is $\frac{\sum \text{ vector lengths}}{\text{no. of vectors}}$. So,

$$\frac{\sum_{k=1}^{\log_2 n} n - 2^{k-1}}{\log_2 n} = \frac{1}{\log_2 n}(n \log n - (n-1)) = \frac{n}{\log n}(\log n - 1) + \frac{1}{\log n} \approx n \left(\frac{\log n - 1}{\log n} \right) \in \bigcirc(n).$$

Performance analysis: Vector $T_v = \tau \log_2 n(S + \frac{n}{2})$. Serial $T_s = Cn$.

$$\lim_{n \to \infty} \frac{T_v}{T_s} = \lim_{n \to \infty} \frac{n \log n}{n} \to \infty.$$

$$\begin{bmatrix} a_1 & b_1 & & & \\ c_2 & a_2 & b_2 & & \\ & c_3 & a_3 & b_3 & \\ & \vdots & \vdots & \vdots & \\ & & & c_8 & a_8 \end{bmatrix}.$$

In Gaussian elimination, $R(2) \leftarrow R_2 - \frac{c_2}{a_1} R_1 - \frac{b_2}{a_3} R_2$ and $R_4 \leftarrow R_4 - c_1 R_2 - c_2 R_6$. Solving for the odd equations is called the *cyclic reduction algorithm.*

Fact: If in some system $Ax = b$, you wish to reorder the equations according to $P^T x$ where P^T is a permutation matrix that satisfies $P^T P = I = P P^T$, then $P^T AX = P^T b$.

$$\begin{aligned} &P^T A(PP^T)x = \ (P^T AP)(P^T x) = P^T b, \\ &A'x' = b', \\ &x' = P^T x \Rightarrow x = Px'. \end{aligned}$$

$$A' = P^T A P = \left[\begin{array}{cccc|cccc} a_1 & & & & b_1 & & & \\ & a_3 & & & c_3 & b_3 & & \\ & & a_5 & & & c_5 & b_5 & \\ & & & a_7 & & & c_7 & b_7 \\ \hline c_2 & b_2 & & & a_2 & & & \\ & c_4 & b_4 & & & a_4 & & \\ & & c_6 & b_6 & & & a_6 & \\ & & & c_8 & & & & a_8 \end{array}\right] \left[\begin{array}{c} x_1 \\ x_3 \\ x_5 \\ x_7 \\ \hline x_2 \\ x_4 \\ x_6 \\ x_8 \end{array}\right] = \left[\begin{array}{c} b_1 \\ b_3 \\ b_5 \\ b_7 \\ \hline b_2 \\ b_4 \\ b_6 \\ b_8 \end{array}\right].$$

$$A' = \left[\begin{array}{c|c} D_1 & F \\ \hline G & D_2 \end{array}\right].$$

$$A\prime = L_1 T_1 U_1 \text{ where } L_1 = \left[\begin{array}{c|c} I & 0 \\ \hline GD_1^{-1} & I \end{array}\right],\ U_1 = \left[\begin{array}{c|c} I & D_1^{-1}F \\ \hline 0 & I \end{array}\right],\ T_1 = \left[\begin{array}{c|c} D_1 & 0 \\ \hline 0 & D_2 - GD_1^{-1}F \end{array}\right].$$

$D_2 - GD_1^{-1}F$ is tridiagonal of length $\frac{n}{2}$.

$$\left[\begin{array}{cccc} c_2 & b_2 & & \\ & c_4 & b_4 & \\ & & c_6 & b_6 \\ & & & c_8 \end{array}\right] \overset{D_1^{-1}}{\left[\begin{array}{cccc} \frac{1}{a_1} & & & \\ & \frac{1}{a_3} & & \\ & & \frac{1}{a_5} & \\ & & & \frac{1}{a_7} \end{array}\right]} = \left[\begin{array}{cccc} \frac{c_2}{a_1} & \frac{b_2}{a_3} & & \\ & \frac{c_4}{a_3} & \frac{b_4}{a_5} & \\ & & \frac{c_6}{a_5} & \frac{b_6}{a_7} \\ & & & \frac{c_8}{a_7} \end{array}\right].$$

$$A' = P_1 A P_1^T = L_1 \left[\begin{array}{c|c} T_{11} & 0 \\ \hline 0 & T_{22} \end{array}\right] U_1,$$

where $A = \overset{=Q}{(P_1^T L_1 P_2^T L_2 \cdots L_k)}\, \overset{=T_k}{T_k}\, \overset{=E}{(U_k P_k U_{k-1} P_{k-1} \cdots P_1)}$, T_k will eventually be a diagonal matrix. Solve $Ax = b = (QT_kE)x = b$, $P_1^T U = r$, $U = P_1 r$. The *perfect shuffle* is used on the permutation matrix P.

$$p = \begin{cases} i \to 2i - 1, & \text{If } i \le \frac{n}{2}. \\ i \to 2i - n, & \text{If } i > \frac{n}{2}. \end{cases}$$

$$\left[\begin{array}{cccc|cccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \hline 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right] \left[\begin{array}{c} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \end{array}\right] = \left[\begin{array}{c} x_1 \\ x_5 \\ x_2 \\ x_6 \\ x_3 \\ x_7 \\ x_4 \\ x_8 \end{array}\right].$$

$$\left[\begin{array}{c} x_1 \\ x_2 \\ x_3 \\ x_4 \end{array}\right] \text{ merge } \left[\begin{array}{c} x_5 \\ x_6 \\ x_7 \\ x_8 \end{array}\right] \text{ using } \left[\begin{array}{c} 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \end{array}\right].$$

$T = \tau\left(58 + \frac{n}{2}\right)$.

$$P^T \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_3 \\ x_5 \\ x_7 \\ x_2 \\ x_4 \\ x_6 \\ x_8 \end{bmatrix}.$$

The problem on the Cray's is that everything is 2 apart (stride = 2). There is no compress instruction. Strides up to 8 or 16 still run good. After 16, the algorithm runs poorly.

Consider the computation $y_i = A_i * B_i + C_i * D_i + 3 * (F_i - G_i) * (G_i + H_i)$, $i = 1, ..., L$. $\frac{L}{S} = 34 + L$. Multiples are $23 + L$. The Voyager timing of y_i is

Instruction	Issue Time	First Result	Last Result
Load F	0	35	$34 + L$
Load G	$34 + L$	69	$68 + 2L$
Subtract $F - G \to V_1$	$68 + 2L$	$91 + 2L$	$90 + 3L$
Load H	$69 + 2L$	$104 + 2L$	$103 + 3L$
Load C	$103 + 3L$	$138 + 3L$	$137 + 4L$
Add $G + H \to V_2$	$104 + 3L$	$127 + 3L$	$126 + 3L$
Multiply $V_1 * V_2 \to V_3$	$126 + 4L$	$149 + 4L$	$148 + 5L$
Load D	$137 + 4L$	$172 + 4L$	$171 + 5L$
Multiply $3 * V_3 \to V_4$	$148 + 5L$	$171 + 5L$	$170 + 6L$
Load A	$171 + 5L$	$206 + 5L$	$205 + 6L$
Multiply $C * D \to V_5$	$170 + 6L$	$193 + 6L$	$192 + 7L$
Load B	$205 + 6L$	$240 + 6L$	$239 + 7L$
Add $V_4 + V_5 \to V_6$	$192 + 7L$	$215 + 7L$	$214 + 8L$
Multiply $A * B \to V_1$	$239 + 7L$	$262 + 7L$	$261 + 8L$
Add $V_1 + V_6 \to y$	$261 + 8L$	$284 + 8L$	$283 + 9L$
Store y	$283 + 9L$	$318 + 9L$	$317 + 10L$

The above operation requires eight floating-point operations.

$F(L) = 8L$,
$T(L) = \tau(317 + 10L)$,
$T(n) = \tau(LSU + \frac{n}{64}(317 + 10(64)) =$
$\tau(LSU + 15n) = 15\tau(\frac{LSU}{15} + n) =$
$(8)\left(\frac{15}{8}\right)\tau\left(\frac{LSU}{15} + n\right) \Rightarrow n_{\frac{1}{2}} = 27 \Rightarrow r_\infty = \frac{1}{\tau\alpha} = \left(\frac{8}{15}\right)240 = 130.$

Homework: Do the above calculation on the Cray-YMP. The answer is similar to $\tau(C + 4L)$. Need at least 7 loads and 1 store. $8(35 + L) = (280 + 8L)$ in the worst case. Take advantage of pipes, chaining, etc.

Example: $c_i = A_i + b_i$. $T(L) = \tau(124 + 4L)$, $L \leq 64$.

$T(n) = \tau(LSU + \frac{n}{64}[124 + 4(64)]) =$
$\tau(LSU + n(2 + 4)) =$
$\tau(LSU + 6n) =$
$6\tau(\frac{LSU}{6} + n) =$
$1(6)\tau(\frac{LSU}{6} + n) =$

$m = 1$. $\alpha = 6$. $n_{\frac{1}{2}} = \frac{LSU}{6}$. $r_\infty = \frac{1}{\tau\alpha} = \frac{1}{6} = 40$ mflops. Use LSU = 400.

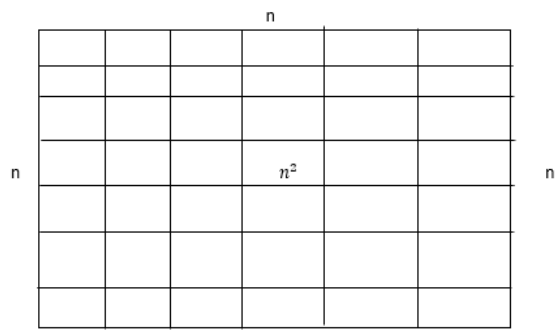


Figure 3.11: This figure shows the example for the grid problem.

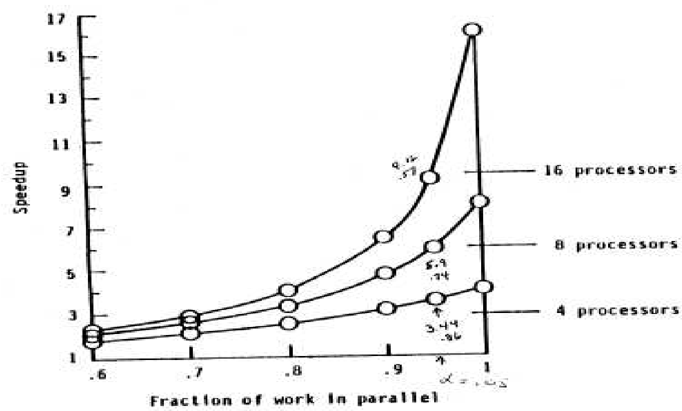


Figure 3.12: This figure shows the speed-up as a function of parallelism and number of processors.

Amdahl's Law

Let α be the fraction of time in a code that cannot be speed-up (vectored or parallelized) by a factor of p when vectored or parallelized. Then, the speed-up is given by

$$S(p, \alpha) = \frac{1}{\alpha + \frac{(1-\alpha)}{p}}$$

where p equals to the number of processors.

Example: Suppose we have a grid problem. See Figure 3.11. $\frac{n}{n^2} \Rightarrow \alpha = \bigcirc(\frac{1}{n})$. The *efficiency* which is the percent on p achieved for given p and α equals

$$\frac{1}{p\alpha + (1-\alpha)}.$$

See Figure 3.12.

User involvement to vectorize an algorithm:

1. None — dust deck runs very well.

2. Minor changes to existing code to increase efficiency. Example: interchanging loops.

3. Minor changes to existing code to allow it to vectorize. Example: break-out offending code.

4. Choosing an effective implementation of an existing algorithm. Example: vectorize the solution of multiple tri-diagonal systems. One tri-diagonal operation does not vectorize. Example: Matrix times vector multiply for a banded matrix.

5. Use or develop a new algorithm to replace the old algorithms. Example: Odd-even reduction for tri-diagonal equations. Example: Recursive doubling to sum a vector.

Suppose we have the following matrix:

$$\begin{bmatrix} a_{11} & a_{12} & & \\ a_{21} & a_{22} & a_{23} & \\ & a_{32} & a_{33} & a_{34} \\ & & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix}.$$

$$\begin{aligned} b_1 &= a_{11}x_1 + a_{12}x_2 \\ b_2 &= a_{21}x_1 + a_{22}x_2 + a_{23}x_3 \\ b_3 &= a_{32}x_2 + a_{33}x_3 + a_{34}x_4 \\ b_4 &= a_{43}x_3 + a_{44}x_4 \end{aligned}$$

$$\begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{21} \end{bmatrix} x_1 + \begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \end{bmatrix} x_2 + \begin{bmatrix} a_{23} \\ a_{33} \\ a_{43} \end{bmatrix} x_3 + \begin{bmatrix} a_{34} \\ a_{44} \end{bmatrix} x_4.$$

Suppose we take an alternate view.

$$\begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{22} \\ a_{33} \\ a_{44} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} + \begin{bmatrix} a_{12} \\ a_{23} \\ a_{34} \end{bmatrix} \begin{bmatrix} x_2 \\ x_3 \\ x_4 \end{bmatrix} + \begin{bmatrix} a_{21} \\ a_{32} \\ a_{43} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}.$$

The schedule for the remainder of the course:

- November 2 — Assign second problem. Paper topic due.
- November 16 — Second problem due.
- November 23 — Oral presentation (3 volunteers).
- November 30 — Remaining presentations. Paper due. Give out exam.
- December 7 — Exam due.

If $F(n) = mn$ where n is the vector length, then $T(n) = \tau(S + \alpha mn)$ where α depends on the architecture. $T(n) = \alpha m\tau(\frac{S}{\alpha m} + n) = \alpha m\tau(C + n) \Rightarrow n_{\frac{1}{2}} = C \Rightarrow r_\infty = \frac{1}{\tau\alpha}$.

3.6 Homework

Instruction	Issue Time	1-st Result	Last Result
Load F	0	20	19+ L
Load G	1	21	20 + L
Subtract $F - G \rightarrow V_1$	21	33	32+L
Multiply $3 * V_1 \rightarrow V_2$	33	46	45+L
Load H	19+L	39+L	38+2L
Load C	20+L	40+L	39+2L
Add $G + H \rightarrow V_3$	39+L	51+L	50+2L
Multiply $V_2 * V_3 \rightarrow V_4$	51+L	64+L	63+2L
Load D	38+2L	58+2L	57+3L
Load A	39+2L	59+2L	58+3L
Multiply $C * D \rightarrow V_5$	63+2L	76+2L	75+3L
Add $V_5 + V_4 \rightarrow V_6$	76+2L	88+2L	87+3L
Load B	57+3L	77+3L	66+4L
Multiply $A * B \rightarrow V_7$	77+3L	90+3L	89+4L
Add $V_6 + V_7 \rightarrow V_1$	90+3L	102+3L	101+4L
Store $V_1 \rightarrow y$	102+3L	122+3L	121+4L

$F(L) = 8L$. $T(L) = \tau(142 + 4L)$. $T(n) = \tau(LSU + \frac{n}{64}(142 + 4(64))) = \tau(LSU + 6.2n) = 6.2\tau(\frac{LSU}{6.2} + n) = 8(\frac{6.2}{8})\tau(\frac{LSU}{6.2} + n)$. For the Cray-YMP, $\frac{1}{\tau} = \frac{1}{6\times10^{-4}\text{ sec}} = 167$ mflops. $r_\infty = (\frac{8}{6.2})167 = 215.5$.

An outline of the source code is as follow:

Dimension U(32, 32)
Integer itmax c max iterations
Float Ax, Bx, Ay, By
Integer Nx, Ny c # x, y grid points
h = 1.0/31.0
Nx = 32
Ny = 32
itmax = 5000
1 Ax = 0.0
Ay = 0.0
Bx = 1.0
By = 1.0
c initialize boundaries
DO 2 J = 1, Ny
x = Ax + **Real**(J-1)*H
2 U(0, J) = 0
U(J, 0) = -3.0*x*x
2 **Continue**

```
DO 3 I = 2, Ny-1
y = Ay + Real(I-1)*H
U(Nx, I) = y*y*y*y - y - 3.0
U(i, Nx) = x - 4.0 *x*x
3 Continue
c initialize array
DO 4 J = 2,Ny-1
y = Ay + Real(J-1)*H
DO 5 I = 2,Nx-1
x = Ax + Real(I-1)*H
U(I, J) = x*y
5 Continue
4 Continue
```

```
HSQ = H*H
DO 6 K=1, Itmax
DO 7 J= 2, Ny-1
y = Ay + Real(J-1)*H
DO 8 I = 2,Nx-1
x = Ax + Real(I-1)*H
v = U(I+1, J) + U(I-1, J) + U(I, J+1) + U(I, J-1)
f = 12.0*y*y*x - 2.0*(y + 3.0) * U(I-1, J-1)
U(I, J) = v / (4.0 - HSQ*f)
8 Continue
7 Continue
6 Continue
Print 9, (U(I, J), I=1, Nx), J=1, Ny)
9 Format(//32(6F13.6)
```

3.7 Homework

This is the matrix multiply programming problem.

Dimensions: arrays A, B, C as nmax x nmax arrays.

Define matrices A and B as follows:

$$A(i,j) = SIN(i+j)$$
$$B(i,j) = COS(i+2*j)$$

where $i, j = 1, ..., nmax$. Perform a matrix by matrix multiplication of A times B for $n = 25,\ nmax,\ 25$ where a) nmax = 200 and b) nmax = 225. For each value of n, compute $C = AB$ using the outer-product by columns, the inner-product, and the outer-product by rows. Print nmax, n, mflops, C(2, 2) for each method. Run your code on Voyager. Turn in the source listing, and the computed results.. Turn in a discussion of the problem and an analysis of the observed performance.

Due date: November 15, 1992.

1. Outer-product by columns.

$$\begin{bmatrix} c_{11} \\ c_{21} \\ c_{31} \end{bmatrix} = \begin{bmatrix} a_{11} \\ a_{21} \\ a_{31} \end{bmatrix} b_{11} + \begin{bmatrix} a_{12} \\ a_{22} \\ a_{33} \end{bmatrix} b_{21} + \begin{bmatrix} a_{13} \\ a_{23} \\ a_{33} \end{bmatrix} b_{31}.$$

2. Inner-product method. $c_{ij} =< (i^{th} \text{ row of } A), (j^{th} \text{ column of } B) >$.

3. Outer-product by rows.

$$
\begin{aligned}
(c_{11}, c_{12}, c_{13}) &= a_{11}(b_{11}, b_{12}, b_{13}) \\
(c_{21}, c_{22}, c_{23}) &= a_{12}(b_{21}, b_{22}, b_{23}) \\
(c_{31}, c_{32}, c_{33}) &= a_{13}(b_{31}, b_{32}, b_{33})
\end{aligned}
$$

3.7.1 Fortran Code

The given problem is to compute the multiplication of two matrices, A and B, and store the result in matrix C. The matrices have the following values: $A(I, J) = \sin(I + J)$, $I, J = 1, nmax$ and $B(I, J) = \cos(I + 2 * J)$, $I, J = 1, nmax$. The three techniques used to compute $A * B$ are:

1. The outer-product by columns.

2. The inner-product.

3. The outer-product by rows.

All three algorithms vectorized. The lengths of the vectors are determined by

DO $n = 1, nmax, 25$

for the two values of nmax equal to 200 and 225. A performance analysis of each algorithm and the source code follows. Figure 3.13 shows the timing.

For the inner-product on the CRAY-YMP, $F(n) = 2n$. $T(n) = \tau[400 + \frac{n}{64}(12 + 2(2)(64)]$, $T(n) = \tau(400 + 4.19n)$, $T(n) = 4.19\tau(95.5 + n)$, $T(n) = 2(\frac{4.19}{2})\tau(95.5 + n)$. $n_{\frac{1}{2}} = 95.5$. $r_\infty = \frac{1}{\tau\alpha} = \left(\frac{2}{4.19}\right)(240) = 115$.

For the outer-product by rows and columns on the CRAY-YMP, $F(n) = n$. $T(n) = \tau(400 + \frac{n}{64}(12 + 128))$, $T(n) = \tau(400 + 2.19n)$, $T(n) = (1)2.19\tau(182.6 + n)$. $n_{\frac{1}{2}} = 182.6$. $r_\infty = \frac{1}{\tau\alpha} = \frac{240}{2.19} = 109.6$.

Some source code is as follow:

1

```
type matrix, f
cat matrix, f
real a(225, 225), b(225, 225), c(225, 225)
real mflop1
real time1
nmax = 225
call initialize(a, b, nmax)
```

```
do 60 nmax = 200, 225, 25
write(6, 200)
do 17 n = 25, nmax, 25
call init_c(c, nmax, n)
c outer product by columns
t1 = second()
do 8 k = 1, n
do 10 i = 1, n
do 15 j=1, n
c(j, k) = a(j, i) * b(i, k) + c(j, k)
15 continue
10 continue
8 continue
t2 = second()
time1 = t2 - t1
mflop1 = 2*real(n**3)/(time1*1.0e+06)
write(6, 100) nmax, n, mflop1, c(2, 2)
17 continue
```

```
c inner-product
call init_c(c, nmax, nmax)
write(6, 300)
do 18 n = 25, nmax, 25
call init_c(c, nmax, n)
t1 = second()
do 27 k = 1, n
do 20 j = 1, n
do 25 i = 1, n
c(j, k) = a(j, i) * b(i, k) + c(j, k)
25 continue
20 continue
27 continue
t2 = second()
time1 = t2 - t1
mflop1 = 2.0*real(n**3)/(time1*1.0e+06)
write(6, 100) nmax, n, mflop1, c(2, 2)
18 continue
```

```
      c outer-product by rows
      call init_c(c, nmax, nmax)
      write(6, 400)
        do 39 n = 25, nmax, 25
        call init_c(c, nmax, n)
        t1 = second()
          do 40 k = 1, n
            do 45 i = 1, n
              do 50 j = 1, n
              c(k, j) = a(k, i) * b(i, j) + c(k, j)
              50 continue
            45 continue
          40 continue
        t2 = second()
        time1 = t2 - t1
        mflop1 = 2.0*real(n**3)/(time1*1.0e+06)
        write(6, 100) nmax, n, mflop1, c(2, 2)
        39 continue
      60 continue
    stop
    100 format(//,'nmax= ',i3,' n= ',i3,' mflops = ',f10.3,' c= 'f10.3,//)
    200 format(//,'outer-product by columns',//)
    300 format(//,'inner-product',//)
    400 format(//,'outer-product by rows',//)
    end
```

```
    subroutine initialize(a, b, nmax)
    real a(nmax, nmax), b(nmax, nmax)
      do 2 i = 1, nmax
        do 1 j = 1, nmax
        a(i, j) = sin(real(i) + real(j))
        b(i, j) = cos(real(i) + 2.0*real(j))
        1 continue
      2 continue
    return
    end
```

```
    subroutine init_c(c, nmax, n)
    real c(nmax, nmax)
      do 4 j = 1, n
        do 5 i = 1, n
        c(i, j) = 0.0
        5 continue
      4 continue
    return
    end
```

Some of the script on Voyager looks like this:

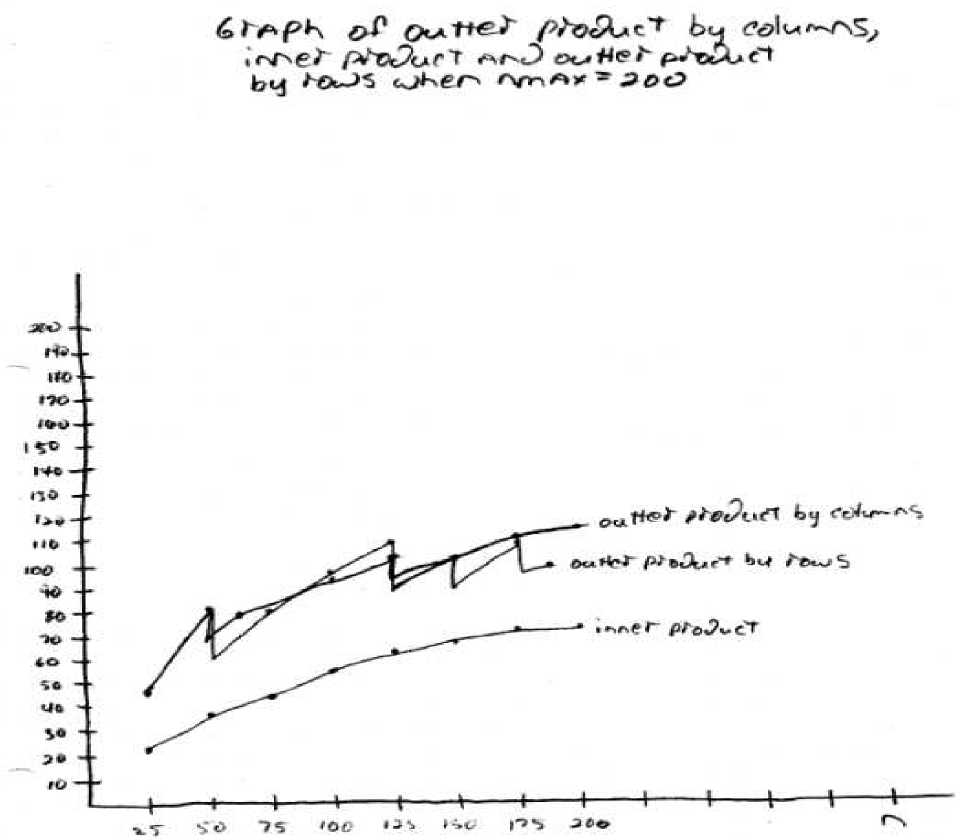


Figure 3.13: This figure shows the "saw-toothed" function for the performance function.

```
voyager %
c> type out.1
cat output
script started on Fri Nov 6 12:18:12 1992
[/dev/ttyp078]
voyager % cft77 -es matrix.f
voyager % segidr -o matrix matrix.o
1 voyager % matrix
....
STOP (called by $Main, line 68)
CP: 5.206s, Wallclock: 42.160s, 3.1% of 4-CPU Machine
voyager % exit
voyager %
Script finished on Fri Nov 6 12:19:38 1992
voyager %
```

The instructor's general comments on this homework problem are as follow:

1. At $n = 64$, should see a "saw-toothed" function for the performance function $f(n)$. See Figure 3.13.

2. The inner-product has considerably lower mflops.

3. The effect of nmax:

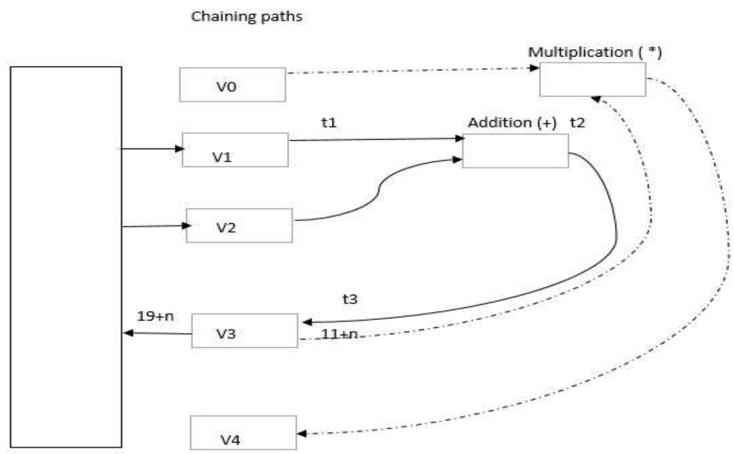


Figure 3.14: This figure shows the memory for chaining paths for the Cray-YMP.

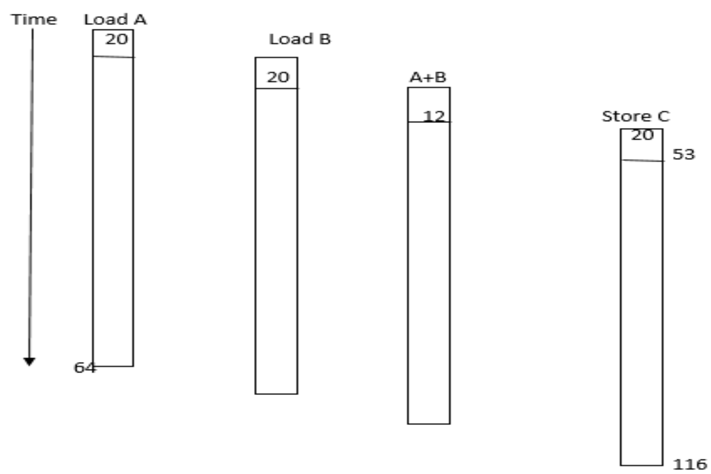


Figure 3.15: This figure shows the timing for chaining paths for the Cray-YMP.

(a) Outer-product by column independent of nmax.

(b) Outer-product by rows is not noticeably affected when nmax = 225.

(c) Reduced performance for other two algorithms when nmax = 200.

(d) Why is the outer-product by rows so low and flat at nmax = 200? Because there are 2 loads and 1 store. $T(L) = \tau(C + 12L)$. $n_{\frac{1}{2}} = \frac{LSU}{14}$ which makes r_∞ low.

3.8 Highlights of the Cray-YMP

- Has up to 8 processors.
- 6 NS clock cycle.
- Has hardware chaining. See Figures 3.14 and 3.15.
- Has 3 ports to memory.
- Has compressed IOTA — gather, scatter.
- Has up to 256 megaword of memory.

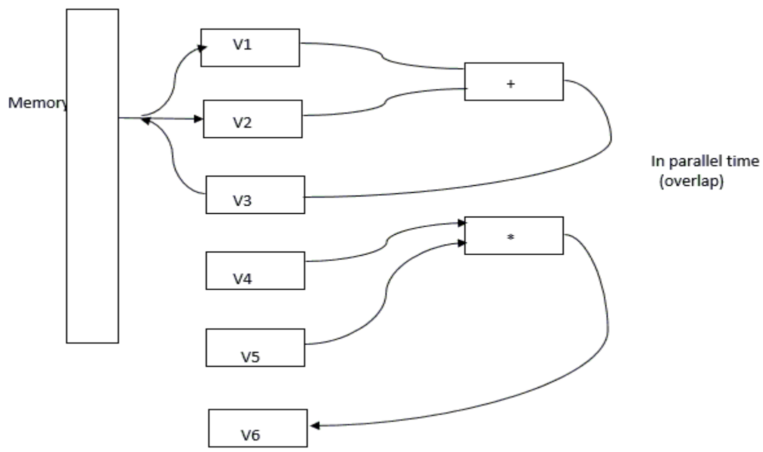


Figure 3.16: This figure shows the swapping of memory in parallel time.

- SSD — 1 gigaword (1,024 megaword).
- I/O subsystem.
  - 4 I/O processors.
  - Local memory.
  - 4 parallel streams per disk controller.
  - 100M byte / sec external channel (HSX).

Sequentially,

Load A	83
Load B	83
$A + B \rightarrow C$	76
Store C	83
	325 Cycles

SSD is dynamic RAM memory. It can be up to 1,024 megawords. The rates to and from memory are 1,000 MB / sec. SSD is used as:

1. Fast disk.

$$1 \left[\begin{array}{l} \text{Write to SSD UKM1} \\ \text{UK} \rightarrow \text{UKM1} \\ \text{UKP1} \rightarrow \text{UK} \\ \text{Read from SSD UKP1} \\ \text{Compute results for UK} \end{array} \right.$$

2. Extended memory — common block of data.
3. Cache for the file system.
4. Swap space.

See Figure 3.16. Two factors affect memory speed:

1. How long is a bank busy? Behavior under a load.

2. How fast data travels to the V registers? Mflop rate is a dedicated system.

Memory cycle time (MCT) is defined as bank busy time. MCT equals to the access time plus the refresh time. Load time equals to the access time plus the travel time.

Example: Suppose MCT equals access time plus refresh time DRAM $= 120 + 110 = 230$. SRAM $= 45 = 45$ $s =$ MCT access time.

Assemble code:

Register	Operation	Comment
V_L	A_k	Transmit (A_k) to V_L
V_i	A_0, A_k	Read V_L words from A_0 with stride $A_k \to V_i$
V_i	$S_j * FV_R$	Floating point multiplication $S_j * V_R \to V_i$
V_m	V_5, P	Set V_m bit to 1 where $V_5 > 0$
V_i	$/HV_j$	$\frac{1}{V_j} \to V_i$
V_i	$V_j * IV_k$	$Z - V_j * V_k \to V_i$
V_i	$V_j!V_k\&V_m$	Merge V_j and V_k using the bit pattern in V_m register and store into V_i

Example:

1 **DO** 3 I = 1, N
  If (C(I).**GT**.0) **Then** A(I) = Exp1
  Else A(I) = Exp2
  Endif
3 **Continue**

Assume $C(I)$ lives in V_3.

1. Evaluate EXP1 $\to V_1$.
2. Evaluate EXP2 $\to V_3$.
3. V_m, V_3, P.
4. $V_4, V!!V_2\&V_m$.
5. $V_4 \to A(I)$.

$$C = \begin{bmatrix} 1 \\ -3 \\ 9 \\ -2 \\ -5 \\ 4 \\ -1 \end{bmatrix} \to V_m \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} \to \text{ Compressed IOTA } \begin{bmatrix} 1 \\ 3 \\ 6 \\ 7 \end{bmatrix}.$$

3.9 Project

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CS 584

CRAY-2 Architecture has no Impact on CNF Satisfiability

Abstract

The Conjunctive Normal Form (CNF) satisfiability problem is the problem of finding boolean assignments to an expression in CNF form such that the expression evaluates to true. A vectored CNF algorithm is presented which loads the boolean truth table into r vector registers. Boolean arithmetic is performed across the registers and the result stored in memory. A sequential algorithm is run on the resulting vector to determine which lines in the truth table made the expression evaluate to true.

The CNF expression contains at most kn operators where k is equal to the number of clauses and n is equal to the number of literals. To evaluate a CNF expression, an exponential amount of time is required despite the CRAY-2 architecture. The evaluation algorithm presented is only executed once to find all the boolean assignments as opposed to an exponential number of times for each line in the truth table. However, the evaluation algorithm presented is still in NTIME due to the exponential length of the vectors.

Introduction

A boolean expression is said to be in CNF form when clauses of "or's" and literals are separated by "and's." An example of a CNF expression would be as follow: $(a + b + -c) * (-a + c) * (a + -b + -c)$. The truth table corresponding to any CNF expression has $n2^n$ entries. The $n2^n$ entries are a listing of every possible boolean combination for each literal. The run-time of the algorithm which builds the truth table is in NTIME.

It is the truth table that is being vectored. A conjunction or a disjunction is performed across 2 registers of length 2^n. A negation is performed across 1 register. The results are stored in memory and brought in for the next calculation. The truth table for the above example looks like this:

i	a	b	c	(a+b+-c)*(-a+c)*(a+-b+-c)	result
0	0	0	0		1
1	0	0	1		0
2	0	1	0		1
3	0	1	1		0
4	1	0	0		0
5	1	0	1		1
6	1	1	0		0
7	1	1	1		1

In the above example, there are three column vectors — one corresponding to each literal. As we will see, the truth table does not have to be extended over the expression. The result after evaluating the expression is given on the right. Note that there are 4 1's in the vector. This means that four lines in the truth table make the expression evaluate to true.

Algorithm 1: Calculate the Truth Table

On a sequential machine, the truth table is generated by converting an integer i into binary form and storing the result in the truth table. A "1" is interpreted as true and a "0" is interpreted as false. The integer i is such that $0 \leq i < 2^n - 1$ and is shown on the far left end of the above example. The truth table need not be computed in its entirety — just one line at a time. This observation will become useful later on. Later on, it will become necessary to identify specific lines in the truth table which made the expression evaluate to true from a column vector.

On a vector machine, it is more desirable to use an algorithm which generates the truth table column by column to increase performance. It will be shown that the evaluation algorithm uses an exponential amount of memory and in thus in NSPACE. The algorithm for constructing the truth table is as follow:

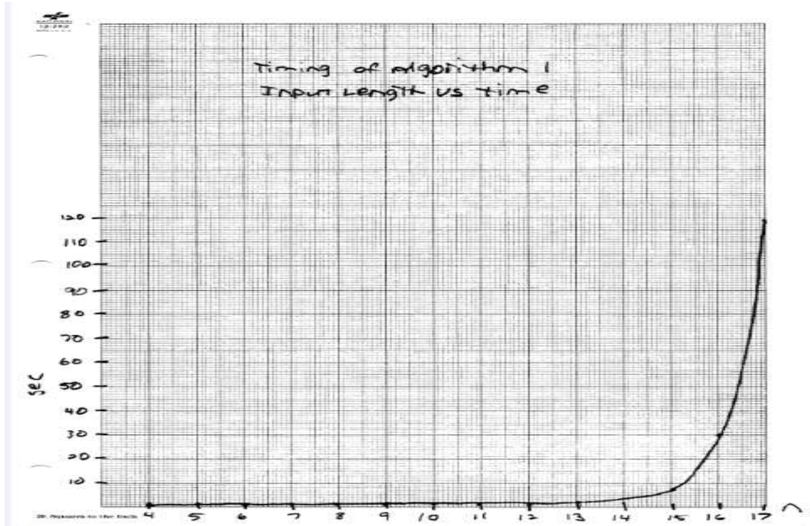


Figure 3.17: This figure shows the timing of Algorithm 1 — n versus time.

Algorithm 1:

```
length = 2^n
  do 1 i = 1, n
  k = 2^i/2
  m = 1
    do 2 j = 1, length
      do 3 p = 1, k
      table(m , i) = false
      m = m + 1
      3 continue

      do 4 p = 1, k
      table(m , i) = true
      m = m + 1
      4 continue
    2 continue
  1 continue
```

See Figure 3.17 for the timing of Algorithm 1 of the size of the problem n versus time. See Figure 3.18 for another timing graph of Algorithm 1 — the size of the problem versus mflops.

Algorithm 2: Infix Notation

In Algorithm 1, the number 1 loop terminates after n iterations. The second do loop terminates after 2^n iterations. Thus, to construct the boolean truth table, we need $n2^n$ iterations. The truth table only needs to be constructed once for all expressions. We can re-use the table over and over again for different expressions since we did not initially extend the table over the expression.

With the boolean truth table in hand, two other algorithms are needed: 1) an algorithm to convert infix expressions into postfix form and 2) an algorithm to evaluate the columns in the truth table according to the expression. When an expression is in postfix form, the evaluation of expressions is facilitated since there

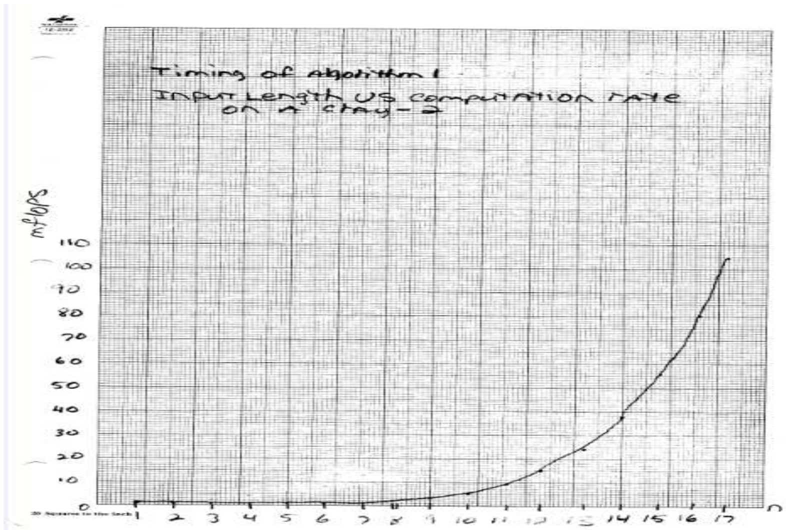


Figure 3.18: This figure shows the timing of Algorithm 1 — n versus mflops.

are no parentheses. The algorithm for converting a boolean expression into postfix notation is as follow:

Algorithm 2:

```
c "last" is the last position in the array infix()
j = 1
1   do 1 i = 1, last
    symb = infix(i)
    if opnd(symb)
        postfix(j) = symb
        j = j + 1
    else
2       while (.not. empty) .and. (prcd(stktop.symb)) do
            call pop(topsymb)
            postfix(j) = topsymb
            j = j + 1
        end while
        if (empty) .or. (symb .ne. ')') call push(symb)
        else call pop(topsymb)
        endif
    endif
    1 continue
c copy remaining symbols into the postfix expression
3   while .not. empty do
        call pop(topsymb)
        postfix(j) = topsymb
        j = j + 1
    end while
```

It is easy to see that the above algorithm will terminate in a polynomial amount of time. The number 1 DO loop will terminate at most after $k(3n-1)+k$ iterations where k is a constant equal to the number of clauses.

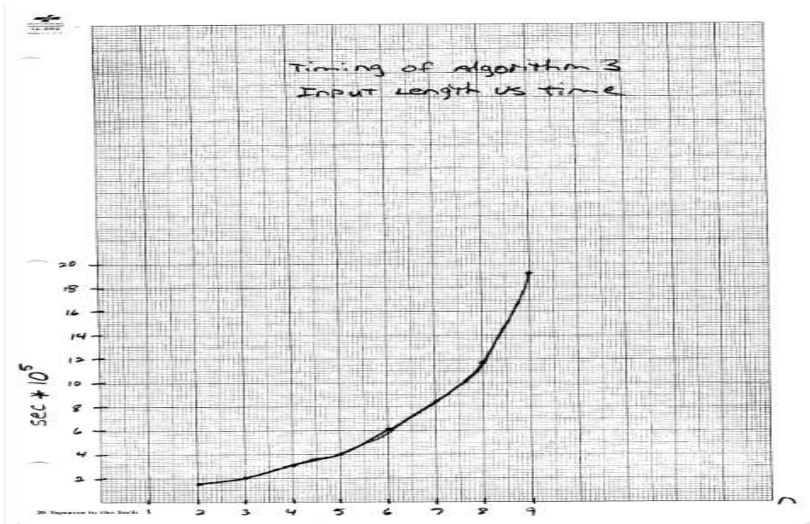


Figure 3.19: This figure shows the timing of Algorithm 3 — n versus time.

Algorithm 3: Evaluation

When an expression is evaluated, for each literal there corresponds a unique arrangement of boolean values that is used throughout the expression. It does not matter which literal gets which column at the start. However, once a decision is made, one must consistently use the same column for a literal throughout the expression. The evaluation algorithm follows:

Algorithm 3:

```
c "last" is the length of the postfix expression
c "length" is the length of the boolean truth table
    do 1 i = 1, last
    symb = postfix(i)
        if opnd(symb) call push(symb)
        else
        call pop(temp)
            if symb .ne. '-' call pop(temp2)
                do 2 j = 1, length
                if symb .eq. '-' table(j.result) = .not. table(j.temp)
                else
                if symb .eq. '*' table(j.result) = table(j.temp) .and. table(j.temp2)
                else
                if symb .eq. "+" table(j.result) = table(j.temp) .or. table(j.temp2)
                2 continue
            end if
        call push(value)
        end if
    1 continue
```

See Figure 3.19 for the timing of Algorithm 3 of the size of the problem n versus time. See Figure 3.20 for another timing graph of Algorithm 3 — the size of the problem versus mflops.

Note that it is the number 2 DO loop which is being vectored. Once the inner DO loop is vectored, there are at most $2n-1$ operations per operand in any clause. There are k clauses. Hence, $k(2n-1)$ operations inside

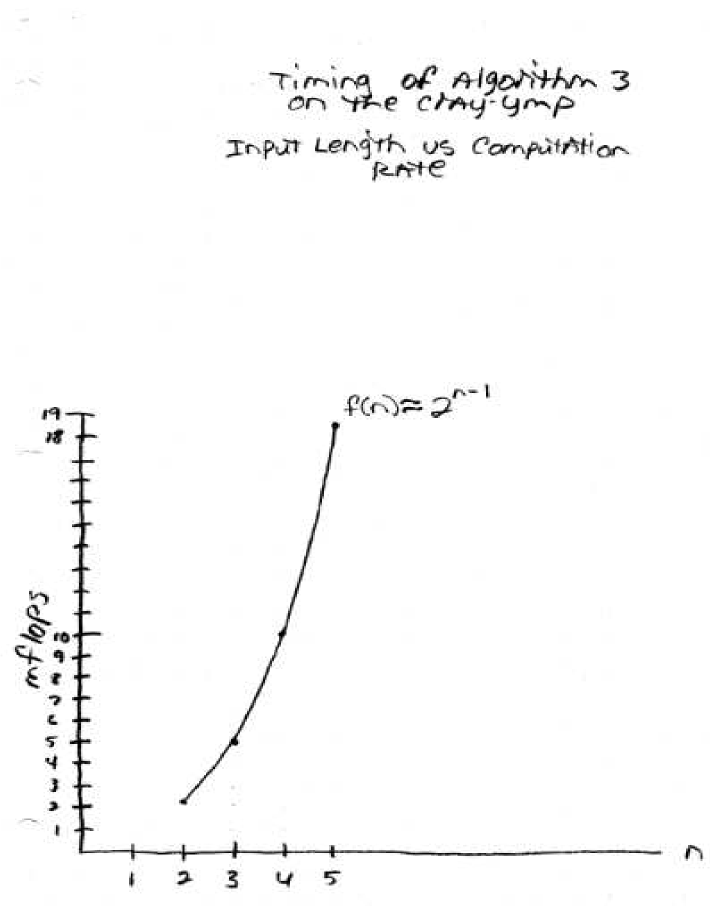


Figure 3.20: This figure shows the timing of Algorithm 3 — n versus mflops.

ar:goodwin

cnfg.f

Mon Nov 30 16:10:51 1992

lw-lpd / LaserWriter

```
lw-lpd ar:goodwin  Job: cnfg.f  Date: Mon Nov 30 16:10:51 1992
lw-lpd ar:goodwin  Job: cnfg.f  Date: Mon Nov 30 16:10:51 1992
lw-lpd ar:goodwin  Job: cnfg.f  Date: Mon Nov 30 16:10:51 1992
lw-lpd ar:goodwin  Job: cnfg.f  Date: Mon Nov 30 16:10:51 1992
```

This is one variation of the program. several variations were used to obtain the graphs in the paper.

Figure 3.21: This figure gives some of the output for the CS 584 Project. Handwritten comments are acceptable.

all clauses. The total number of "and's" outside the parentheses is $k-1$. The most number of operations to be performed is $k(2n-1)+(k-1)$. Each vector is 2^n in length. Hence, $\bigcirc(kn2^n)$ algorithm.

A programming trick that was used in Algorithm 3 replaces all literals with an integer valued index into the boolean truth table. It not only ensures that the number 2 DO loop is vectored, but it also facilitates looking-up columns in the table corresponding to some literal.

Conclusion

The architecture of the CRAY-2 had no impact on the CNF satisfiability problem. It does allow us to solve larger instances of the problem at faster rates. However, architecture is not a substitute for problem solving. The successful algorithms on the CNF problem take advantage of problem characteristics and certain data structures.

Fortran Code

Figure 3.21 shows some of the printout for this project. Noted, the instructor did have comments.

```
logical table(8192, 19)
integer length
real time1, mflop1, t1, t2
integer temp, temp2, r, flag, tp2
integer pop, a(100), top
integer postfix(100)
integer last, m
n = 10
top = 0
c read input expression
    do 70 i= 1, 19
    read *, postfix(i)
    70 continue
last = 19
```

```
c compute the boolean truth table
length = ifix((2.0**n)
t1 = second()
    do 1 i = 1, n
    k = ifix(2.0**i/2.0)
    m = 1
        do 2 j = 1, length
            do 3 p = 1, k
            table(m, i) = .false.
            m = m+1
            3 continue
            do 4 p = 1, k
            table(m, i) = .true.
            m = m+1
            4 continue
        2 continue
    1 continue
t2 = second()
time1 = t2 - t1
mflop1 = 3.0*real(n)*real(length)/(time1*10e+06)
write(6, 100) time1
```

```
      c the evaluation algorithm
      r = n+1
      t1 = second()
          do 20 i = 1, last
          symb = postfix(i)
          flag = opnd(symb)
              if (flag .eq. 1) then
              call push(s, top, symb)
              else
              temp = pop(s, top)
   7          if (symb .ne. 24) tp2 = pop(s, top)
      8           do 25 j = 1, length
                  if (symb .eq. 24) table(j, r) = .not.table(j, temp)
1        9        if (symb .eq. 23) table(j, r) = table(j, temp).and.table(j, tp2)
                  if (symb .eq. 22) table(j, r) = table(j, temp).or.table(j, tp2)
                  25 continue
              call push(s, top, r)
              end if
          20 continue
      t2 = second()
      time1 = t2 - t1
      mflop1 = 3.0*real(last)*real(length)/(time1*1.0e+06)
      write(6, 100) time1
      100 format(//,'seconds = ', f15.8,//)
      200 format(//,i1,i1, i2//)
      300 format(//,i2,//)
      stop
      end

      function opnd(symb)
          if ((symb .ge. 1).and.(symb .le. 18)) then
          opnd = 1
1  10     else
          opnd = 0
          end if
      return
      end

      subroutine push(s, top, c)
      integer s(100), top, c
1     top = top+1
      s(top) = c
      return
      end

      integer function pop(s, top)
      integer s(100), top
1     pop = s(top)
      top = top - 1
      return
      end
```

Project References

1. Chao, Ming-Te and John Franco, "Probabilistic Analysis of Two Heuristic for the 3-Satisfiability Problem," *SIAM Journal on Computing,* Volume 15, pp 1106-118, 1986.

2. Franco, John and Marvin Pauli, "Probabilistic Analysis of the Davis-Putnam Procedure for Solving the Satisfiability Problem," *Discrete Applied Mathematics,* Volume 5, pp. 77 - 87, 1983.

3. Iwama, Ka Zua, "CNF Satisfiability Test by Counting and Polynomial Average Time," *SIAM Journal on Computing,* Volume 18, pp. 385 - 91, 1989.

4. NASA, *CRAY,* NASA Technical Memorandum 107599, Document CX-1c, Mini Manual, April 1992.

5. Purdom, P. and C. Brown, "Polynomial Average Time Satisfiability Problems," *Information Science,* Volume 41, pp. 23 - 42, 1983.

3.10 Final Exam

1. Determine r_∞ and $n_{\frac{1}{2}}$ for:

   (a) A linked triad on a 4-pipe CYBER-205 when 32-bit arithmetic is used.

   (b) Same computer as above, but for the computation $a_i = \frac{b_i}{c_i} + d_i - e_i$, $i = 1, ..., n$. Use a table.

   (c) A succession of 3 vector multiplies and 3 vector additions on our CRAY-2 which gives (you may presume) a timing of $T = \tau(300 + 5m)$ when $m \doteq 64$.

   (d) Same computation as in (c), but for a CRAY-like computer with a 2 nsec clock, vector registers of length 128, and an LSU value of 200.

2. The $N \times N$ matrix A is symmetric and banded. The semi-bandwidth is S. That is, there are S non-zero super diagonals and sub-diagonals, as well. Define the variable $W = S + 1$. Assume that the main and super diagonals are stored as columns of the FORTRAN array ABAND, where ABAND is dimensioned ABAND(N, W) according to the following rule: $A_{I,J} \rightarrow ABAND(I, J - I + 1)$. Write a stride 1 program that computes $b = Ax$ for any value N or S. Assume that A and x are already initialized. You may use CYBER-205 vector syntax or regular CRAY FORTRAN.

3. In general, what would be the effect on r_∞ and $n_{\frac{1}{2}}$ if the computer manufacturer did the following things to his architecture? Treat each of those below as independent of the others in this exercise.

   (a) Halved the minor cycle time on the CYBER-205.

   (b) Halved the start-up time on the CYBER-205.

   (c) CRAY reduces the size of vector registers to 32 words.

   (d) CRAY halves the start-up time for each of their vector instructions. For instance, an instruction with timing like $22 + m$ is reduced to $11 + m$.

4. Over the years, the Control Data Corporation CYBER-205 and CRAY X-MP were two main supercomputer architectures. However, CRAY has prevailed and CDC no longer is in the supercomputer business. Describe the important attributes of the two computers, emphasizing the features of the two computers that explain the downfall of one and the success of the other.

5. In class, we manipulated the timing equation for a computation which has an operation count of the form $F(n) = mn$ to give us the equation of a straight line from which we could graphically determine r_∞ and $n_{\frac{1}{2}}$. In the above, F is the total number of floating-point operations and n is the vector length.

   (a) Use a similar approach to define the straight line equation that allows us to determine r_∞ and $n_{\frac{1}{2}}$ when the computation has an operation count of the form $F(n) = f(n)n$.

(b) Use the timings from the last programming problem to graphically estimate r_∞ and $n_{\frac{1}{2}}$ for the matrix multiplication outer-product by columns on the CRAY-2. Provide the graph, with values plotted also.

6. Given the equation $E_i = A_i B_i + C_i D_i$, $i = 1, ..., n$ determine r_∞ and $n_{\frac{1}{2}}$ for:

   (a) A 4-pipe CYBER-205 using 64-bit arithmetic.

   (b) The CRAY-2.

   (c) The CRAY-YMP.

7. A vector algorithm to compute $S = \sum_{i=1}^{n} a_i$ can be constructed as follows: Perform a vector add of length $\frac{n}{2}$ on the top half of the array to the bottom half, giving $\frac{n}{2}$ results. One can then repeat the procedure on that result array. Only it is half as big now, and continue until one has the single value S. Assuming that n is of the form $n = 2^k$:

   (a) What is the average vector length?

   (b) What is the timing formula (2-pipes, 64-bit, CYBER-205)?

   (c) Is the algorithm consistent? Why or why not?

Please sign a pledge that states you neither gave nor received help on this exam.

I will pick up the exam in the corridor outside our room on Friday, December 11 at 4:30. Feel free to turn it in before then if you are finished.

Good luck!

3.11 Course References

1. Lambiotte, Jay, "Architecture and Performance of SNS Computers Presentation," Computer Applications Branch, October 1991.

2. NASA, *CONVEX,* NASA Technical Memorandum 107564, Document CX-1e, Mini Manual, February 1992.

3. NASA, *CRAY,* NASA Technical Memorandum 107599, Document CX-1c, Mini Manual, April 1992.

4. NASA, *Introduction to the LaRC Central Scientific Computing Complex,* NASA Technical Memorandum 104092, Document A-1e, April 1991.

5. NASA, *SNS Programming Environment User's Guide,* NASA Technical Memorandum 107565, Document A-8a, February 1992.

Chapter 4

Stochastic Models in Computer Science

Dr. Simha, College of William and Mary

CSCI 524, Fall 1991

Text used: Solomon, Frederick, *Probability and Stochastic Processes,* Prentice Hall, 1987

4.1 Stochastic vs Non-stochastic Approaches

Find the expected income from rental of a pier. A non-stochastic approach is to get the schedule for the year(not reliable information) and compute the total rent. A stochastic approach is to compare the schedule with the previous year's data; take samples from last year's data; find the average number of ships per day; multiply $\bar{x}$ by the rental fee per day by 365.

Differences

Non-stochastic	Stochastic
Assumes full knowledge	Postulate from last year's data
Large amount of data	Small amount of data
Large cancellation	Easy calculation
If the data is accurate, then the answer is accurate	At best, a guess

When data is impossible to obtain, a stochastic method must be used. Why study stochastic modeling in computer science?

- Useful in evaluating designs(algorithms, architectures).
- Modeling system behavior(operating systems).
- Computational aspects of stochastic modeling.
- Theoretical foundation.

4.2 Review

4.2.1 Review of Sets

Sets: union and intersection. Only infinite set will be used. $\{1, 2, 3, ...\} = \aleph$, the set of natural numbers. $\{..., -3, -2, -1, 0, 1, 2, 3, ...\} = Z$, the set of integers. $Q = \frac{a}{b}, a, b \in Z, b \neq 0$, is the set of rational numbers(finite length). $\Re$ is the set of real numbers(infinite length). The *cardinality* is the size of sets, denoted by $||$.

4.2.2 Review of Sequences

A sequence is a collection of real numbers indexed by natural numbers. Formally, a mapping of: $\aleph \to \Re$. $1.3, 2.3, 3.3, ... : a_n = n + .3$. Generally, sequences $a_1, a_2, a_3, ..., a_n$. If $a_n = \frac{1}{n}$, then $\lim_{n\to\infty} a_n = 0$. Limits may or may not be in the sequence given. Suppose, $a_n = 1 - \frac{1}{n}$. Then, $\lim_{n\to\infty} a_n = 1$. Definition: $\lim_{n\to\infty} a_n = L$, iff for every $\epsilon > 0, \exists N(\epsilon)$, such that the following is true: $\forall n > N(\epsilon), |a_n - L| < \epsilon$.

Example: Suppose $|a_n - 0| = \left|\frac{1}{n} - 0\right| = \frac{1}{n}$. $e = 0.01, \frac{1}{101}, \frac{1}{102}, \frac{1}{103}, ...$

Prove the following two expressions:

$$\lim_{n\to\infty} \frac{1}{n} = 0.$$

$$\lim_{n\to\infty} \frac{1}{n} \neq 0.001.$$

Given $e > 0$, which $n's$ satisfy

$$\left|\frac{1}{n} - 0\right| < e?$$

Only if, $n > \frac{1}{\epsilon}$. By taking $N(\epsilon) = \frac{1}{\epsilon}$, we know $\forall n > N(\epsilon)$,

$$\left|\frac{1}{n} - 0\right| < \epsilon$$

Prove the second equation:

$$\lim_{n\to\infty} \frac{1}{n} \neq 0.001.$$

Proof: Suppose the limit is true. Then, $\exists \bar{N}(\epsilon)$ function. Given $\epsilon > 0, \forall n > \bar{N}(\epsilon)$,

$$\left|\frac{1}{n} - 0.001\right| < \epsilon.$$

Choose $\epsilon = 0.0005$. Pick n larger than

$$\max\left(\bar{N}(0.0005), \frac{1}{0.0005}\right).$$

Then $\frac{1}{n'} < 0.0005$. Therefore,

$$\left|\frac{1}{n'} - 0.001\right| > 0.0005 = \epsilon.$$

Example: $a_n = 1$. So, $1, 1, 1, 1, ... \lim_{n\to\infty} 1 = 1$. $N(\epsilon) = 1$.

Example: $a_n = (-1)^n$. $-1, +1, -1, +1, ... \lim_{n\to\infty} -1^n \neq 1$, for any L. For $N(\epsilon)$, pick $\epsilon = 0.5, N(0.5)$. Do not choose $\epsilon = 10$. It's too big.

4.2.3 Combinations of Sequences

Suppose, $a_n \to a$, and $b_n \to b$. Let $c_n = a_n + b_n$. Then, $c_n \to a + b$. $\lim_{n\to\infty} c_n = \lim_{n\to\infty} a_n + b_n = a + b$. To prove use the limit definition and construct a and b.

Example: $a_n = \frac{1}{n}; b_n = 1 + \frac{1}{n}$. $a_n \to 0$. $b_n \to 1$. So, $c_n = 1 + \frac{1}{n} + \frac{1}{n} = 1 + \frac{2}{n} = 1$. Similarly, $a_n - b_n \to a - b$, $a_n b_n \to ab$, $\frac{a_n}{b_n} \to \frac{a}{b}$. $ca_n \to ca$, where c is a constant.

4.2.4 Limits and Functions

$f : \Re \to \Re$, eg $f(x) = x^2$. Suppose $x_1, x_2, ..., x_n$ is a sequence such that $x_n \to \bar{x}$. Then, $f\left(\lim_{n\to\infty} x_n\right) = f(\bar{x})$. Next, let $y_n = f(x_n)$. Then, $y_1, y_2, ..., y_n$ is a sequence. Does $y_n \to f(\bar{x})$? Not true when $f(\bar{x})$ is discontinuous. $f(x) = x^2$. $x_n = 3 + \frac{1}{n}$. So, $x_n \to 3 = \bar{x}$. $y_n = f(x_n) = x_n^2 = 9 + \frac{6}{n} + \frac{1}{n^2}$. $y_n \to 9 = f(\bar{x})$.

Example:

$$f(x) = \begin{cases} 0, & \text{if } 0 \leq x \leq 3. \\ x^2, & \text{if } x > 3. \end{cases}$$

$x_n = 3 + \frac{1}{n}$. So, $x_n \to 3 = \bar{x}$. Thus, $f(\bar{x}) = 0$. But, $y_n = 9$.

4.2.5 Sequences of Functions

$f_1(x), f_2(x), ...$ Each $f_n : \Re \to \Re$.

Example:

$$f_n(x) = x^2 + \frac{1}{n}.$$

Choose $x = 3$. Then, $f_1(3), f_2(3), ... = 9 + 1, 9 + \frac{1}{2}, 9 + \frac{1}{3}, ..., 9 + \frac{1}{n}$. So, $f_n(3) \to 9$, $f_n(4) \to 16$. More generally, $f_n(x) \to x^2$. $f_n(x) = f(x) = x^2$.

4.2.6 Sums and Averages

Given a sequence $a_1, a_2, a_3, ...$ construct:

1. The sequence of partial sums. $b_1 = a_1$. $b_2 = a_1 + a_2 ....$ $b_n = a_1 + a_2 + ... + a_n$.

$$\sum_{i=1}^{n} a_i.$$

2. The sequence of partial averages. $c_1 = a_1$. $c_2 = \frac{(a_1 + a_2)}{2} ....$ $c_n = \frac{a_1 + \cdots + a_n}{n} =$

$$\frac{1}{n} \sum_{i=1}^{n} a_i.$$

Example:

$$a_n = \left(\frac{1}{2}\right)^n, \; b_n = \sum_{i=1}^{n} \left(\frac{1}{2}\right)^i, \; c_n = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{1}{2}\right)^i.$$

Let $a_n = x^n, 0 < x < 1$. $b_n = x + x^2 + \cdots + x^n = \frac{x}{1-x}(1-x^n)$. $a_n \to 0$. $b_n \to \frac{x}{1-x}$. $\lim_{n\to\infty} b_n = \lim_{n\to\infty}\sum_{i=1}^n a_i = \sum_{i=1}^n a_i$.

Partial averages. Suppose $a_n = 5$. $5, 5, 5, ...$ $a_n \to 5$.

$$c_n = \frac{a_1 + \cdots + a_n}{n} = \frac{5n}{5} = 5.$$

So, $c_n \to 5$. Suppose that

$$a_n = \begin{cases} 5, & \text{if } n \text{ is even.} \\ 6, & \text{if } n \text{ is odd.} \end{cases}$$

$a_n = 6, 5, 6, 5, ...$ a_n converges to nothing. $c_n \to 5.5$.

$$a_n = \begin{cases} 5, & \text{if } n \text{ is even.} \\ 6, & \text{if } n \text{ is odd.} \end{cases}$$

$$c_n = \frac{a_1 + \cdots + a_n}{n} = \frac{1}{n}\left[\left(\frac{n}{2}\right)6 + \left(\frac{n}{2}\right)5\right], n \text{ even.}$$

$$\frac{1}{n}\left[\left(\frac{n+1}{2}\right)6 + \left(\frac{n-1}{2}\right)5\right], n \text{ odd.}$$

$$c_n \to \begin{cases} \frac{6+5}{2}, & \text{if } n \text{ is even.} \\ \frac{6+5}{2} + \frac{1}{2n}, & \text{if } n \text{ is odd.} \end{cases}$$

$c_n \to \frac{6+5}{2} = 5.5$.

Example: Toss a fair coin. Obtain \$1.00 if heads, \$0.00 dollars otherwise. Repeat the experiment n times. What is the average win?

$$\frac{1 + 1 + 0 + 1 + \cdots + 0 + 1}{n} = c_n$$

$c_n \to \frac{1}{2}$. That is, the probability of obtaining heads.

4.2.7 Other Forms of Limits

1. Instead of writing $a_n = \frac{1}{n}$, write $a(n) = \frac{1}{n}$.
2. Sometimes a superscript is used.
$$\lim_{n\to\infty} a_x^{(n)}.$$
3. Sometimes the sequence is not specified.
$$\lim_{x\to 3} f(x).$$
4. Sometimes one out of several variables is taken in a limit.
$$f(x, y, n) = x + \frac{y}{n}.$$
5. The notation $\sum_{i=1}^{\infty} a_i$ will be used for series.

4.3 Basic Probability

Some terminology.

1. *experiment* - or single observation which can be performed at least in thought, any number of times under the same relevant conditions. Examples include: tossing a coin, drawing a card from a deck.
2. *sample space* - the set of possible outcomes or results or observations.
3. *event* - a subset of the sample space, Ω.

If A is an event and $W \in A$ occurs, we say that 'A occurred.' $\Omega \subseteq \Omega$. $\emptyset \subseteq \Omega =$ the empty set. $\{1\}, \{2\}, ...$ are *elementary events.*

Example: A coin flip. $\Omega = \{H, T\}$. Events are $\{H\}$, and $\{T\}$. An experiment would be 3 coin flips. An example of an outcome from an experiment: $\{HHHTTTH\}$. In general there are $2^{|\Omega|}$ unique combinations.

4.3.1 Discrete and Continuous Sample Spaces

A discrete sample space is a countable set such:

1. Finite.
2. Some cardinality as $|\aleph|$.

$\Re$ is an example of an uncountable set. Some examples:

- $\{1, 2, 3, 4, 5, 6\} = \Omega$ is discrete and finite.
- $\{1, 2, 3, ...\} = \Omega$ is discrete and infinite.
- $[12.3, 169.45]$ is continuous and uncountably infinite. This can refer to height, weight, time of day, etc.

Probabilities are *numbers* associated with *events.* Given a sample space, Ω, a *probability measure* is a collection of real numbers, one for each event A in Ω. $P(A)$ for A which satisfy:

1. $P(\Omega) = 1$.
2. $0 \leq P(A) \leq 1$ for every $A \subseteq \Omega$.
3. For disjoint events $A, B \subseteq \Omega$, $P(A \cup B) = P(A) + P(B)$.

Example: A coin flip. $\Omega = \{H, T\}$. $\emptyset : P(\emptyset) = 0$. $\{H\} : P(\{H\}) = \frac{1}{2}$. $\{t\} : P(\{T\}) = \frac{1}{2}$. $\{H, T\} : P(\{H\}) + P(\{T\}) = 1$.

Example: Throwing a die. $\Omega = \{1, 2, 3, 4, 5, 6\}$.

Events	Number
$\emptyset$	$P(\emptyset) = 0$
$\{1\}$	$P(\{1\}) = \frac{1}{6}$
.	.
.	.
.	.
$\{6\}$	$P(\{6\}) = \frac{1}{6}$
$\{1, 2\}$	$P(\{1, 2\}) = \frac{2}{6}$
.	.
.	.
.	.

In general, for any event $\{x_1, ..., x_k\} \subseteq \{1, 2, ..., k\}$. Define $P(\{x_1, ..., x_k\}) = P(\{x_1\}) + \cdots + P(\{x_k\})$. Axioms 1-3 stated above are satisfied. A *distribution* is a way in which you describe the probability.

4.3.2 Some Basic Properties

1. Consider $A, B \subseteq \Omega$, such that $A \subseteq B$. Then, $B - A = P(B) - P(A)$. proof: $B = A \cup (B - A)$. $P(B) = P(A) + P(B - A)$.

2. For $A \subseteq \Omega$, define $A^c = \Omega - A$. Then, $P(A^c) = 1 - P(A)$. proof: $A \cup A^c = \Omega$. $P(\Omega) = P(A) + P(A^c)$. $1 = P(A) + P(A^c)$.

3. $A_1, ..., A_n$ are *disjoint events.* Then,
$$P\left(\bigcup_{i=1}^{n} A_i\right) = \sum_{i=1}^{n} P(A_i).$$

4. $A, B \subseteq \Omega$ *not necessarily disjoint events.* Then, $P(A \cup B) = P(A) + P(B) - P(A \cap B)$. proof: $A \cup B = [A - (A \cap B)] \cup [B - (A \cap B)] \cup (A \cap B)$. $P(A \cup B) = P(A) - P(A \cap B) + P(B) - P(A \cap B) + P(\cap B) = P(A) + P(B) - P(A \cap B)$.

Example: A die throw. Suppose we want P(result is an odd number). $\Omega = \{1, 2, 3, 4, 5, 6\}$. Event $A = \{1, 3, 5\}$. $P(\{i\}) = \frac{1}{6}, i = 1, 2, 3, 4, 5, 6$. $P(\{1, 3, 5\}) = P(\{1\}) \cup P(\{3\}) \cup P(\{5\}) = \frac{1}{6} + \frac{1}{6} + \frac{1}{6} = \frac{1}{2}$.

4.3.3 Countable Additivity

Consider an infinite sequence of events $A_1, A_2, A_3, ...$ where each $A_i \subseteq \Omega$.

Example: $\Omega = \{1, 2, 3, 4, ...\}$ $A_1 = \{1, 2\}, A_2 = \{2, 3\}$ etc.

Replace axiom 3 with: Suppose $A_1, A_2, ...$ are disjoint. Then,
$$P\left(\bigcup_{i=1}^{\infty} A_i\right) = \sum_{i=1}^{\infty} P(A_i).$$

Example: $\Omega = \{1, 2, 3, ...\}$. $A_1 = \{1\}, A_2 = \{2\}, ..., A_n = \{n\}$. Suppose that $P(\{n\}) = \frac{1}{2^n}$. Then,
$$\bigcup_{I=1}^{\infty} A_i = \Omega.$$
$$P(\Omega) = P\left(\bigcup_{i=1}^{\infty} A_i\right) = \sum_{i=1}^{\infty} P(A_i) = \sum_{i=1}^{\infty} \frac{1}{2^i} = \frac{1}{2} + \frac{1}{2^2} + \frac{1}{2^3} + \cdots = \frac{\frac{1}{2}}{1 - \frac{1}{2}} = 1.$$

Example: A complex experiment. 3 coin flips, 1 die throw, and 1 card drawing. $\Omega_1 = \{H, T\}$, $\Omega_2 = \{H, T\}$, $\Omega_3 = \{H, T\}$, $\Omega_4 = \{1, 2, 3, 4, 5, 6\}$, $\Omega_5 = \{A_s, ..., K_d\}$.

To find the cross product of sets given 2 sets $A = \{a_1, ..., a_n\}$ and $B = \{b_1, ..., b_m\}$. $A \times B = \{(x, y) : x \in A, y \in B\} = \{(a_1, b_1), ..., (a_n, b_m)\}$. As an example: $N_o = \{1, 3, 5, ...\}; N_e = \{2, 4, 6, ...\}$. $N_o \times N_e = \{(x, y) : x, y \in \aleph, x$ is odd, y is even.

In the previous example, $\Omega = \Omega_1 \times \Omega_2 \times \Omega_3 \times \Omega_4 \times \Omega_5 = \{(x_1, x_2, x_3, x_4, x_5) : x_i \in \Omega_i\}$. eg: $(H, T, H, 3, A_d) \in \Omega$, is called an outcome of the experiment.

Look for sources of randomness to break-down an experiment.

Example: Two die throws is a complex experiment. The elementary experiments are the first throw and the second throw. $\Omega_1 = \{1, 2, 3, 4, 5, 6\}; \Omega_2 = \{1, 2, 3, 4, 5, 6\}$. $\Omega = \Omega_1 \times \Omega_2 = \{(x, y) : x \in \Omega_1, y \in \Omega_2\}$. eg. $A = \{(1, 1), (2, 2), (3, 3)\}$ is an event of the experiment.

$A \subseteq \Omega$	$P(A)$
$\{(1,1)\}$	$\frac{1}{6}\frac{1}{6} = \frac{1}{36}$
$\{(1,2)\}$	$\frac{1}{6}\frac{1}{6} = \frac{1}{36}$
.	.
.	.
.	.
$\{(6,6)\}$	$\frac{1}{6}\frac{1}{6} = \frac{1}{36}$
.	.
.	.
.	.

4.4 Homework and Answers

1. Consider the sequence $a_n = \frac{4n}{5+3n}$ and answer the following:

   (a) Show informally that $a_n \to \frac{4}{3}$.

   $$\lim_{n\to\infty} \frac{4n}{5+3n} = \lim_{n\to\infty} \frac{\frac{4n}{n}}{\frac{5+3n}{n}} = \lim_{n\to\infty} \frac{4}{\frac{5}{n}+3} = \frac{4}{0+3} = \frac{4}{3}.$$

   (b) Provide a formal proof of the same thing using the definition of a limit, i.e., construct the $N(\epsilon)$ function for this case.

   $$\left|\frac{4n}{5+3n} - \frac{4}{3}\right| < \epsilon,$$

   $$\left|\frac{12n - 4(5+3n)}{15+9n}\right| < \epsilon,$$

   $$\left|\frac{12n - 20 - 12n}{15+9n}\right| < \epsilon,$$

   $$\left|\frac{-20}{15+9n}\right| < \epsilon.$$

   Carry out the division and solve for n. Set $N(\epsilon) = n$.

   (c) Show that a_n does not converge to zero. Show that any $N(\epsilon)$ function fails to work.

2. A speeding vehicle is ticketed by a police officer, who notes the license plate number(consisting of six characters). Assuming we are interested in observing the plate number, identify the sample space and

the event corresponding to "the license plate contains at least three A's."

The sample space is constructed as follow: $\Omega_1 = \{a, b, c, ..., z\}$. $\Omega_2 = \{a, b, c, ..., z\}$. $\Omega_3 = \{a, b, c, ..., z\}$. $\Omega_4 = \{a, b, c, ..., z\}$. $\Omega_5 = \{a, b, c, ..., z\}$. $\Omega_6 = \{a, b, c, ..., z\}$. $\Omega = \Omega_1 \times \Omega_2 \times \Omega_3 \times \Omega_4 \times \Omega_5 \times \Omega_6$. $\Omega = \{(x, y, z, t, u, w) : x \in \Omega_1, y \in \Omega_2, z \in \Omega_3, t \in \Omega_4, u \in \Omega_5, v \in \Omega_6$ and three letters are 'A.'$\}$

It is assumed that license plates contain all characters and no numbers.

3. A fair coin is tossed once and its outcome is observed. If the outcome is 'heads,' the coin is tossed again and the outcome recorded. Write down the sample space for this experiment. Is it a complex experiment? Can it be naturally decomposed into more elementary experiments? If so, is the sample space expressible as a cross-product? Give an example of an event. Assign a probability measure and compute(with explanation) the probability of obtaining two 'heads.'

   The sample space is: $\Omega = \{HH, HT, T1, ..., T6\}$. Yes, the experiment is a complex experiment in that there are 2 sources of randomness — flipping a coin and throwing a die. The experiment can be decomposed into two separate sample spaces. $\Omega_1 = \{H, T\}$. $\Omega_2 = \{T, 1, ..., 6\}$. $\Omega = \Omega_1 \times \Omega_2 = \{(x, y) : x \in \Omega_1; y \in \Omega_2; (T, y) : y \in \{1, ..., 6\}\}$ An example of an event would be $A = \{(HT), (T1)\}$. The probability of $\{(TT)\}$ is zero since it is not part of the sample space. The probability of $\{(HH)\}$ is given as follow: $A =$ 1-st flip is heads. $B =$ 2-nd flip is heads. $P(B|A) = \frac{1}{2}$. $P(A) = \frac{1}{2}$. $P(A \cap B) = P(B|A)P(A) = \left(\frac{1}{2}\right)\frac{1}{2} = \frac{1}{4}$.

4. Let Ω be any finite sample space with n elements, i.e., $|\Omega| = n$. For each event $A \subseteq \Omega$, define $P(A) = \frac{|A|}{n}$. Show that this association of numbers with events is a valid probability measure(show that the three axioms are satisfied). Give an example of an experiment for which this would be a suitable probability measure.

   By definition, $P(\Omega) = \frac{|\Omega|}{n} = \frac{n}{n} = 1$.

4.5 Programming Assignment

This is a short programming assignment designed to get you comfortable with infinite sequences of real numbers. In this programming assignment, you will study sequences of real numbers to determine if certain types of limits exist. For an infinite sequence of real numbers $a_1, a_2, a_3, ...$ (each a_i is a *term* or *element* of the sequence) one is often interested in answering the following questions:

1. Does the sequence $a_1, a_2, a_3, ...$ converge to any limit, i.e., do terms in the sequence appear to get closer to any particular number, and if so, what is that number?

2. Construct a new sequence $b_1 = a_1, b_2 = a_1 + a_2, ..., b_n = \sum_{i=1}^{n} a_i, ...$ Does the sequence of *partial sums* $b_1, b_2, b_3, ...$ converge to any limit?

3. Construct yet another sequence $c_1 = a_1, c_2 = \frac{a_1+a_2}{2}, ..., c_n = \frac{1}{n}\sum_{i=1}^{n} a_i, ...$ Does this sequence of *partial averages* converge to anything?

You are given some code which will produce terms from three sequences from which you are to find answers to the above questions *for each of the three different sequences.* This is implemented as a PASCAL **function get_from_sequence(i: integer)** which will return the next term in the i-th sequence ($i = 1, 2, 3$) when called. Thus, if we denote the first two terms of the third sequence as a1 and a2 then they may be obtained as follows:

- start_over;
- get_from_sequence(3);

- get_from_sequence(3);

The procedure **start_over** ensures that the first call to **get_from_sequence** (following a call to **start_over**) generates the very first term in the sequence. Thus, to get the first two elements once again, it is necessary to call **start_over** before using **get_from_sequence.**

Deliverables for this assignment:

You should hand in two neat copies(one for my records) of:

- Supporting documentation for the program: a paragraph describing your code.
- A complete listing of your code together with procedures I have supplied. Your code will contain copious in-line documentation, of course.
- Annotated output from your program. For each sequence:
  1. Print the first 20 terms.
  2. Print the 100th term of the sequence, the 100th term in the corresponding sequence of partial sums and partial averages.
  3. Do the same for the 10000th terms of the sequence, the sequence of partial sums, and partial averages.
- What do the various sequences(and the constructed sequences of partial sums and partial averages) appear to converge to? Can you argue that these are the limits for the sequence?

Note:

- Use at least 6 decimal places of accuracy when printing real numbers.
- Do not confuse the sequence number with the subscript of a particular element or with constructed versions of a particular sequence. Thus, the 2-nd sequence($i = 2$ in **get_from_sequence(i)**) has its first, second, third,..., etc terms. Corresponding sequences of partial sums and partial averages are constructed using terms entirely from the 2-nd sequence. Thus the three sequences each have two additional constructed sequences which you must consider.
- You may write your program in C if you like.
- You are encouraged to play around with the sequences to see what convergence behavior they demonstrate.
- This is NOT a long assignment. You should not need more than 50(text) lines of code.
- Have fun!

```
program first_assignment (input, output);
const
     m = 2147483647; (* const used in random # generator *)
     num_proc = 10;
var
    p,s: array[0..num_proc] of real;
    x_seed: integer;
    index_A, index_B: integer;
```

```
(*......................................................*)
(* Random number generator                              *)

function x_random: real;
const
     a = 16807;
     q = 127773;
     r = 2836;
var
     t,lo,hi: integer;
begin
     hi:= x_seed div q;
     lo:= x_seed - q*hi;
     t:= a*lo - r*hi;
     if (t>0) then
          x_seed:= t
     else
          x_seed:= t+m;
     x_random:= x_seed/m;
end;

(*......................................................*)
(* initialize the random number generator               *)

procedure put_seed(x: integer);
begin
     if (0<x) and (x<m) then x_seed:= x;
end;

(*......................................................*)
(* Reset all sequences                                  *)

procedure start_over;
begin
     put_seed(7774755);
     index_A:= 1;
     index_B:= 1;
end;

(*......................................................*)

procedure initialize;
var
     i: integer;
begin
     start_over;
     p[0]:= 0.4;
     s[0]:= p[0];
     for i:= 1 to num_proc do
     begin
          p[i]:= 0.6/num_proc;
          s[i]:= s[i-1] + p[i];
     end;
end;
```

```
(*....................................................*)
(* This function returns the next term in the specified sequence*)

function get_from_sequence(x: integer):real;
var
     i: integer;
     u: real;
begin
     case x of
          1: begin
                  get_from_sequence:= 1-1/sqr(index_A);
                  index_A:= index_A + 1;
             end;
          2: begin
                  get_from_sequence:= 1/index_B;
                  index_B:= index_B + 1;
             end;
          3: begin
                  u:= x_random;
                  i:= 0;
                  while (u>s[i]) and (i<10) do
                     i:= i + 1;
                  get_from_sequence:= i;
             end;
      end;
end;

(*....................................................*)
(* main program - insert your code here. You may break your code*)
(* into several procedures/functions.                        *)

procedure terms(sqnc: integer);
var
     i: integer;
     n: real;
begin
     start_over;
     writeln(outfile, 'The first 20 terms of sequence',sqnc:2, ' are: ');
     for i:= 1 to 20 do
     begin
          n:= get_from_sequence(sqnc);
          writeln(outfile, n:8:6);
     end;
     for i:= 21 to 100 do get_from_sequence(sqnc);
     writeln(outfile);
     writeln(outfile);
     writeln(outfile);
     write(outfile, 'The 100-th term of sequence',sqnc:2,' = ');
     writeln(outfile, n:12:6);
     writeln(outfile);
     for i:= 101 to 10000 do n:= get_from_sequence(sqnc);
     write(outfile,'The 10000-th term of sequence',sqnc:2,' = ');
     writeln(outfile,n:18:16);
```

```
     writeln(outfile);
     writeln(outfile);
     writeln(outfile);
end;

procedure partial_sums(sqnc: integer);
var
     i: integer;
     n: real;
     k: real;
     writeln(outfile, ' The first 20 terms of partial sums of sequence',
        sqnc:2,' are ');
     for i:= 1 to 20 do
     begin
          n:= get_from_sequence(sqnc);
          k:= k+n;
          writeln(outfile, k:8:6);
     end;
     for i:= 21 to 100 do
     begin
          n:= get_from_sequence(sqnc);
          k:= k+n;
     end;
     writeln(outfile);
     writeln(outfile);
     writeln(outfile);
     write(outfile,'The 100-th term of partial sums of sequence',
        sqnc:2,' = ',k:12:6);
     writeln(outfile);
     for i:= 101 to 10000 do
     begin
          n:= get_from_sequence(sqnc);
          k:= k+n;
     end;
     writeln(outfile);
     writeln(outfile);
     write(outfile,'The 10000-th term of partial sums of sequence',
        sqnc:2,' = ',k:12:6);
     writeln(outfile);
     writeln(outfile);
     writeln(outfile);
end;

procedure partial_averages(sqnc: integer);
(* the following procedure computes the partial average of a given
sequence *)
var
     i: integer;
     n: real;
     k: real;
     m: integer;
begin
     start_over;
     k:= 0.0;
```

```
     writeln(outfile, 'The first 20 terms of partial averages of sequence',
        sqnc:2,' = ');
     m:= 1;
     while n<=20 do
     begin
          for i:= 1 to m do
          begin
               n:= get_from_sequence(sqnc);
               k:= k+n;
          end;
          k:= k/i;
          writeln(outfile, k:8:6);
          m:= m+1;
          start_over;
          k:= 0.0;
     end;
     for i:= 1 to 100 do
     begin
          n:= get_from_sequence(sqnc);
          k:= k+n;
     end;
     writeln(outfile);
     writeln(outfile);
     k:= k/i;
     write(outfile,'The 100-th term of partial averages of sequence',
        sqnc:2,' = ',k:12:6);
     start_over;
     k:= 0.0;
     for i:= 1 to 10000 do
     begin
          n:= get_from_sequence(sqnc);
          k:= k+n;
     end;
     writeln(outfile);
     writeln(outfile);
     k:= k/i;
     write(outfile,'The 10000-th term of partial averages of sequence',
        sqnc:2,' = ',k:24:22);
     writeln(outfile);
     writeln(outfile);
     writeln(outfile);
     writeln(outfile);
end;


(*......................................................*)
begin
   initialize;
   for i:= 1 to 3 do
   begin
        terms(i);
        partial_sums(i);
        partial_averages(i);
   end;
```

`end.`

Sequence 1 Here $a_n = 1 - \frac{1}{n^2}$. As $n \to \infty$, $\frac{1}{n^2} \to 0$ and so $a_n \to 1$. A more formal proof would use $N(\epsilon) = \epsilon^{\frac{1}{2}}$, but you were not required to provide this. Next, consider the sequence of partial sums $b_n = \sum_{i=1}^n a_i$. One may decompose each term in the sequence of partial sums into two parts: $b_n = \sum_{i=1}^n a_i = n - \sum_{i=1}^n \frac{1}{i^2}$. Any decent calculus textbook will(should) tell you that $\sum_{i=1}^n \frac{1}{i^2}$ converges. It happens to converge to $\frac{\pi^2}{6}$. So the second part of our decomposition gets closer and closer to the constant $\frac{\pi^2}{6}$. You might have discovered this for yourself by printing out the latter sum and observing the convergence. The first part diverges. Since, for any constant c, the sequence $n + c \to \infty$, we must have $b_n \to \infty$. Finally, consider the sequence of partial averages $c_n = \frac{1}{n}\sum_{i=1}^n a_i$. Again, the same decomposition gives us: $c_n = \frac{1}{n}\sum_{i=1}^n a_i = 1 - \frac{1}{n}\sum_{i=1}^n \frac{1}{i^2}$. Since the latter sum converges to a constant, $\sum_{i=1}^n \frac{1}{i^2}$ gets closer to $\frac{\pi^2}{6}$ for large n. Hence $\frac{1}{n}\sum_{i=1}^n \frac{1}{i^2}$ will converge to zero. Thus, $c_n \to 1$. Formal proofs for the last two cases are slightly more complicated and were not required.

Sequence 2 The second sequence is $a_n = \frac{1}{n}$. We have seen that $a_n \to 0$ already. Again, your calculus book would tell you that the sequence of partial sums, $b_n = \sum_{i=1}^n \frac{1}{i}$ diverges, although it's not experimentally obvious. It's not very difficult to show divergence by expressing the sum as an integral. It can be shown that $b_n \geq \ln(n+1) + C_1$, for some constant C_1. Since $\ln(n+1)$ diverges, b_n, diverges. It can also be shown that $b_n \leq \ln(n) + C_2$ where C_2 is also a constant. Thus for each term in the sequence of partial averages is less than $\frac{\ln(n)+C_2}{n}$ and so the sequence of partial averages converges to zero. Most of the arguments were for sequence 1; I did, however, take off a few points for a complete lack of reasoning or very wrong answers.

Sequence 3 This sequence is random, as most of you observed. The sequence itself and the sequence of partial sums do not converge. However, the sequence of partial averages will appear to converge to 3.3. Limits for random sequences are treated a little differently, as we shall see later. The sequence of partial averages does indeed converge to 3.3, but in different sense than for real sequences. You were not expected to mention this — I only took off points for incorrect observations.

4.6 Card Experiments

Example: 51 cards, throw one out, say the king of spades. Again, let $A = \{\text{card is a spade}\}$, $B = \{\text{card is an ace}\}$. $P(A|B) = \frac{P(A\cap B)}{P(B)}$. $P(B|A) = \frac{P(A\cap B)}{P(A)}$. $A = \{1, ..., 12\}$, and $B = \{1, 14, 27, 40\}$. Find, $\frac{P(\{1,...,12\})\cap P(\{1,14,27,40\})}{P(\{1,14,27,40\})} = \frac{\frac{1}{51}}{\frac{4}{41}} = \frac{1}{4}$. $P(B|A) = \frac{\frac{1}{51}}{\frac{12}{51}} = \frac{1}{12}$. $P(A) = \frac{12}{51} \neq P(A|B)$. $P(B) = \frac{4}{51} \neq P(B|A)$.

Example: A first card is drawn and not replaced. A second card is drawn. Let A= "1-st card is ace of spades," and B= "second card is two of spades." $\Omega_1 = \{1, ..., 52\}$, and $\Omega_2 = \{1, ..., 52\}$. $\Omega = \{(x, y) : x \in \Omega_1, y \in \Omega_2 \text{ and } x \neq y\}$. $A = \{(1, y) : y \in \Omega_2, y \neq 1\}$. $B = \{(x, 2) : x \in \Omega_1, x \neq 2\}$. $P(A) = \frac{1}{52}$ $P(B) = P(\text{2nd card is 2}|\text{1st card is 1}) = \frac{1}{51}$. $A \cap B = \{(1, 2)\}$. $P(A \cap B) = P(B|A)P(A) = \frac{1}{52}\frac{1}{51}$. $P(\{x, y\}) = \frac{1}{52(51)}, x \neq y$. $P(B) = P(\{(i, 2)) : i \in \Omega, i \neq 2\}) = P(\{(1, 2), (3, 2), (...), (52, 2)\} = P(\{(1, 2)\} + \cdots + P(\{(52, 2)\}) = \frac{1}{51(52)} + \cdots + \frac{1}{52(51)} = \frac{1}{52}$.

Example: A urn has 3 red balls and 2 blue balls. Pick two balls without replacement. Let A='both are the same color.' Find $P(A)$. $\Omega_1 = \{R, B\}$, $\Omega_2 = \{R, B\}$. $\Omega = \{(R, R), (R, B), (B, R), (B, B)\}$ $A = \{(R, R), (B, B)\}$ The probability measure, $P(\text{1-st is red}) = \frac{3}{5}$. $P(\text{1-st is blue}) = \frac{2}{5}$. $P(\text{2-nd is red}|\text{1-st is red}) = \frac{2}{4}$. $P(\text{2-nd is blue}|\text{1-st is blue}) = \frac{1}{4}$. $P(\text{2-nd is red}|\text{1-st is blue}) = \frac{3}{4}$. $P(\text{2-nd is blue}|\text{1-st is red}) = \frac{2}{4}$. $P(\{(R, R)\}) = P(\text{1-st red} \cap \text{2-nd red}) = P(\{(R, B), (R, R)\} \cap \{(R, R), (B, R)\}) = P(\text{2-nd red} \mid \text{1-st red})P(\text{1-st red}) = \frac{2}{4}\frac{3}{5} = \frac{6}{20}$. $P(\{(R, B)\}) = P(\text{2-nd blue} \mid \text{1-st red})P(\text{1-st red}) = \frac{2}{4}\frac{3}{5} = \frac{6}{20}$. $P(\{(B, B)\}) = \frac{2}{20}$. $P(A) = P(\{(R, R), (B, B)\}) = P(\{(R, R)\}) + P(\{(B, B)\}) = \frac{6}{20} + \frac{2}{20} = \frac{8}{20}$.

Example: 3 card draw without replacement. $A = \{\text{1-st card spade}\}$, $B = \{\text{2-nd card spade}\}$, $C = \{\text{3-rd card spade}\} = P(A \cap B \cap C) = P((A \cap B) \cap C) = P(C|A \cap B)P(A \cap B) = P(C|A \cap B)P(B|A)P(A) = \frac{11}{50}\frac{12}{51}\frac{13}{52}$.

4.7 Conditional Probability

Example: 2 card drawing. Draw the first card and do not replace it. Draw another card. $\Omega_1 = \{1, ..., 52\}$, $\Omega_2 = \{1, ..., 52\}$. $\Omega = \{(x, y) : x \in \Omega_1; y \in \Omega_2, x \neq y\}$. eg $(3, 3) \notin \Omega$.

Example: Examine the CPU of a multiuser machine. Count the number of users logged on. Count the number of batch jobs. Count the number of interactive jobs. $\Omega_1 = \{1, 2, 3, ..., n\}$, $\Omega_2 = \{1, 2, 3, ..., n\}$, $\Omega_3\{1, 2, 3, ..., n\}$. $\Omega = \Omega_1 \times \Omega_2 \times \Omega_3 = \{(0, x, y) : y > 0\}$.

Example: Two die throws (independent experiment). $P(\{i, j\}) = P(\{i\})P(\{j\})$, $i, j \in \{1, 2, 3, 4, 5, 6\}$, where $P(\{i\}) = \frac{1}{6}$.

Example: Toss a coin(dependent experiment). If heads, set second toss to tails; else set second toss to heads. $\Omega = \{(H, T), (T, H)\}$. $P(\{H, T\}) = \frac{1}{2} \neq P(\{H\})P(\{T\})$.

Example: A single die throw(conditional probability). $\Omega = \{1, 2, 3, 4, 5, 6\}$. Let $A = \{1, 6\}$, and $B = \{5, 6\}$. $P(A) = P(\{1\}) + P(\{6\}) = \frac{1}{6} + \frac{1}{6} = \frac{1}{3}$. Repeat the experiment n times. Let $f_A(n)$ be the number of times A occurs. Let $f_B(n)$ be the number of times B occurs. Look at $\frac{f_A(n)}{n} \to \frac{1}{3} = P(A)$. Suppose we know that B occurred. What is the probability that A occurred also? Note that for both A and B to occur, $A \cap B$. Let $f_{A\cap B}(n)$ be the number of times both A and B occurs. Then, $\frac{f_{A\cap B}(n)}{f_B(n)} = \frac{\frac{f_{A\cap B}(n)}{n}}{\frac{f_B(n)}{n}} \to \frac{P(A\cap B)}{P(B)} = P(A|B)$. $P(A|B) = \frac{P(A\cap B)}{P(B)}$. In the example, $P(A|B) = \frac{P(A\cap B)}{P(B)} = \frac{\{1,6\}\cap\{5,6\})}{P(\{5,6\})} = \frac{P(\{6\})}{P(\{5,6\})} = \frac{\frac{1}{6}}{\frac{2}{6}} = \frac{1}{2}$.

Example: Draw a card. Let A be that the card is a spade. Let B be that the card is an ace. $\Omega = \{1, ..., 52\}$. $A = \{1, ..., 13\}$, and $B = \{1, 14, 27, 40\}$. Find $P(A|B)$. $P(\{i\}) = \frac{1}{52}, i \in \{1, ..., 52\}$. $P(A|B) = P(\text{spade}|\text{ace}) = \frac{P(A\cap B)}{P(B)} = \frac{P(\{1\})}{P(\{1,14,27,40\})} = \frac{\frac{1}{52}}{\frac{4}{52}} = \frac{1}{4}$. $P(B|A) = P(\text{ace}|\text{spade}) = \frac{P(A\cap B)}{P(A)} = \frac{P(\{1\})}{P(\{1,...,13\})} = \frac{\frac{1}{52}}{\frac{13}{52}} = \frac{1}{13}$. Notice that $P(A|B) = P(A)$. Events A and B are independent iff $P(A \cap B) = P(A)P(B)$, $P(A|B) = P(A)$, and $P(B|A) = P(B)$. $P(A|B) = \frac{P(A\cap B)}{P(B)} = \frac{P(A)P(B)}{P(B)} = P(A)$.

4.8 Law of Total Probability

Let Ω be a sample space. $B_1, B_2, ..., B_n$ is a partition of Ω if

1. $B_i \cap B_j = \emptyset$.
2. $\bigcup_{i=1}^{n} B_i = \Omega$.

The law of total probability for $A \subseteq \Omega$, $P(A) = P((A\cap B_1) \cup ... \cup (A\cap B_n)) = P(A\cap B_1) + ... + P(A\cap B_n) = P(A|B_1)P(B_1) + ... + P(A|B_n)P(B_n)$.

Example: Two card draw without replacement. Let A be that the 'second card is an ace.' If B_1 is 'first card is an ace,' and B_2 is 'first card is not an ace.' Then, $P(A) = P(A|B_1)P(B_1) + P(A|B_2)P(B_2) = \frac{3}{51}\frac{4}{52} + \frac{4}{51}\frac{48}{52}$.

Example: A factory has three machines. Machine A produces 20% of the products. Machine B produces 30% of the products. Machine C produces 50% of the products. For machine A, 6% of the products are defective. For machine B, 7% of the products are defective. For machine C, 8% of the products are defective. Select a product randomly and let E be the event that the product is defective. What is $P(E)$? $S_A =$ product made by A, $S_B =$ product made by B, $S_C =$ product made by C. $P(S_A) = 0.2$, $P(S_B) = 0.3$, $P(S_C) = 0.5$. $P(E|S_A) = 0.06$, $P(E|S_B) = 0.07$, $P(E|S_C) = 0.08$. $S_A \cup S_B \cup S_C \cup = \Omega$. $S_A \cap S_B = \emptyset$. $P(E) = P(E|S_A)P(S_A)+P(E|S_B)P(S_B)+P(E|S_C)P(S_C) = (0.06)(0.2)+(0.07)(0.3)+(0.08)(0.5)$. As an alternative, let $\Omega_1 = \{A, B, C\}$. $\Omega_2 = \{D, N\}$. $\Omega = \Omega_1 \times \Omega_2$. $P(\{(A, D)\}) = P(\text{defect}|\text{made on A})P(\text{made on A}) = P(E|S_A)P(S_A)$. $P(S_A|E) + \frac{P(S_A \cap E)}{P(E)} = \frac{0.06(0.2)}{(0.06)(0.2)+(0.07)(0.3)+(0.08)(0.5)} = \frac{P(E|S_A)P(S_A)}{P(E)}$.

4.9 General Form of Baye's Formula

Suppose $B_1, ..., B_n$ is a partition of Ω. To get $P(B_i|A)$:

1. First compute $P(A) = \sum_{i=1}^{n} P(A|B_i)P(B_i)$.
2. Then, $P(B_i|A) = \frac{P(A|B_i)P(B_i)}{P(A)}$.

Example: There are 2 types of people: accident prone(30% of the population), and non-accident prone(70% of the population). For an accident prone person, $P(\text{accident}) = 0.4$. For a non-accident prone person, $P(\text{accident}) = 0.2$. Compute the probability a person will have an accident and given a person who has an accident, what is $P($ person is accident prone$)$. Let $A =$ person is accident prone, $B =$ person is not accident prone, $C =$ person has an accident. $P(A) = 0.3$, $P(B) = 0.7$, $P(C|A) = 0.4$, $P(C|B) = 0.2$. For the first question: use the law of total probability since the conditions hold true. $P(C) = P(C|A)P(A) + P(C|B)P(B) = (0.4)(0.3) + (0.2)(0.7) = 0.26$. For the second question: $P(A|C) = \frac{P(C|A)P(A)}{P(C)} = \frac{(0.4)(0.2)}{0.26}$.

Example: A plane crashes. It can be in one of 3 regions(equally likely). If the plane is in region i, what is the probability of locating it? Call this α_i. Given that a search in region 1 is unsuccessful, that is the probability it is in region $i, i = 1, 2, 3$? Let $A_i =$ plane is in region i. Let $B_i =$ search of region i is successful. $P(A_i) = \frac{1}{3}$. $P(B_i|A_i) = \alpha_i$. Find $P(A_i|B_1^c)$.

$i = 1:$ $P(A_1|B_1^c) = \frac{P(B_1^c|A_1)P(A_1)}{P(B_1^c)} = P(B_1^c) = P(B_1^c|A_1)P(A_1) + P(B_2^c|A_2)P(A_2) + P(B_3^c|A_3)P(A_3) = \frac{(1-\alpha_1)\frac{1}{3}}{(1-\alpha_1)\frac{1}{3}+(1(\frac{1}{3}))+(1(\frac{1}{3}))}$.

$i = 2:$ .....

4.10 Independence

Events A and B are *independent* if $P(A \cap B) = P(A)P(B)$. If A and B are independent, then so are:

1. A, B^c.
2. A^c, B.
3. A^c, B^c.

4.11 Homework

1. There are two urns. The first contains 3 white balls and 6 red balls whereas the second contains 2 white balls and 9 red balls. A ball is selected from the first urn and dropped into the second. After this, a

ball is drawn from the second urn. What is the probability that the ball is white? $\Omega_1 = \{Red, White\}$. $\Omega_2 = \{Red, White\}$. $\Omega = \{(x, y) : x \in \Omega_1; y \in \Omega_2\}$. Let A = select a white ball from urn 1. B = slect a red ball from urn 1. C = select a white ball from urn 2. $A = \{(W, 0)\}$, $B = \{(R, 0)\}$, $C = \{(W, W), (R, W)\}$. $P(A) = \frac{3}{9} = \frac{1}{3}$. $P(B) = \frac{6}{9} = \frac{2}{3}$. $P(C) = P(\{(W, W)\} + P(\{(R, W)\}$. $P(C|A) = \frac{3}{12} = \frac{1}{4}$. $P(C|B) = \frac{2}{12} = \frac{1}{6}$. $P(C) = P(C|A)P(A) + P(C|B)P(B) = \left(\frac{1}{4}\right)\frac{1}{3} + \left(\frac{1}{6}\right)\frac{2}{3} = 0.194$. The law of total probabilities holds true.

2. In its quest to stop the spread of certain diseases, the government decides to actively encourage people to undergo a blood test. The effectiveness of the blood test is described as follows. For a person with the disease, the test returns "positive" with probability x. For a healthy individual, the test returns "positive"(a false positive) with probability y. The actual fraction of the population with the disease is z. Next, let u be the probability that a randomly selected individual tests positive, d be the conditional probability that the individual has the disease given that he/she tested positive and h be the conditional probability that the individual is healthy given that he/she test positive.

   (a) Express u, d and h as functions of x, y and z.

   (b) Calculate u, d and h when:

      i. $x = 0.95, y = 0.03$, and $z = 0.5$.

      ii. $x = 0.95, y = 0.03$, and $z = 0.1$.

      iii. $x = 0.95, y = 0.03$, and $z = 0.01$.

   Do the results surprise you? What do you conclude? Give an intuitive explanation of the results.

3. Three shady characters, A, B and C are picked up from the streets of New York and taken to court. One of them, A, is charged with a crime and the other two are to be witnesses(they know the truth). The probability that A is guilty is 0.8. Now, B and C testify in sequence. Since B is a friend of $A's$, B will tell the truth if A is innocent, but will lie with probability 0.2 if A is guilty. On the other hand, C dislikes A and will tell the truth if A is guilty but will lie with probability 0.3 if A is innocent.

   (a) Identify the sample space and draw a tree representing the conditional probabilities.

   (b) What is the probability that the witnesses give conflicting testimony?

   (c) Which witness is more likely to commit perjury?

   (d) What is the conditional probability that A is innocent, given that B and C give conflicting testimony?

4. A computer center has two machines, A and B, each with an attached hard disk. Machine A is considered unusable if either it or its attached hard disk fails. The same holds for machine B. Let a_0 be the probability that machine A fails, and a_1 the probability that its hard disk fails; similarly, let b_0 be the probability that machine B fails and b_1 be the probability that its hard disk fails. Assume all failures are independent. The center is closed if both machines are unusable. Compute the probability that the center is closed. Given that the center is closed, what is the probability that a failure of $A's$ hard disk contributed to the closure?

4.12 More on Independence

Example: A parallel machine with n processors, each with probability of failure of q. What is the probability that at least one processor is usable? $1 - q^n$. Let A_i = i-th processor failed.

$$P(\text{all processors failed}) = P(A_1 \cap A_2 \cap \cdots \cap A_n) = P(A_1)P(A_2)\cdots P(A_n) = q^n.$$

Example: A urn has r red balls, g green balls, and b blue balls. Balls are drawn with replacement until either a red or green ball appears. What is the probability that of getting a red ball before a green ball? Let A_n be the event that 'a red ball is drawn on the n-th draw.' Let B_n be the event that 'a blue ball is drawn on the n-th draw.' Let C_n be the event that 'the first red ball on the n-th draw.' Let E_n be the event that 'a red ball is drawn before a green ball.' Then, $E = C_1 \cup C_2 \cup C_3 \cup \cdots \cup C_n$.

$$P(E) = P(C_1 \cup C_2 \cup C_3 \cup \cdots \cup C_n) = P(C_1) + P(C_2) + P(C_3) + \cdots + P(C_n).$$

$$P(C_n) = B_1 \cap B_2 \cap B_3 \cap \cdots \cap B_{n-1} \cap A_n = P(B_1 \cap B_2 \cap B_3 \cap \cdots \cap B_{n-1} \cap A_n) =$$
$$P(B_1)P(B_2)P(B_3) \cdots P(B_{n-1})P(A_n).$$

Let $p = \frac{r}{r+g+b} = P(A_n)$ and $q = \frac{b}{r+g+b} = P(B_n)$. Then, $P(C_n) = (1-p-q)^{n-1}p$. So,

$$P(E) = \sum_{i=1}^{\infty}(1-p-q)^{n-1}p = \frac{p}{p+q} = \frac{r}{r+g}.$$

$A_1, ..., A_n$ are independent events if for every group of $k \leq n$ events among $A_1, ..., A_n$, $P(A_{n_1}) \cap P(A_{n_2}) \cap \cdots \cap P(A_{n_k}) = P(A_{n_1})P(A_{n_2}) \cdots P(A_{n_k})$. It is not enough for events to be pairwise independent.

Example: Select an integer from $\{1, 2, 3, 4\}$ randomly. Let $A_1 = \{1, 2\}$, $A_2 = \{1, 3\}$, $A_3 = \{1, 4\}$. $P(A_1) = \frac{1}{2}$, $P(A_2) = \frac{1}{2}$, $P(A_3) = \frac{1}{2}$. $P(A_1 \cap A_2) = P(\{1\}) = \frac{1}{4}$, $P(A_1 \cap A_3) = P(\{1\}) = \frac{1}{4}$, $P(A_2 \cap A_3) = P(\{1\}) = \frac{1}{4}$, $P(A_1 \cap A_2 \cap A_3) = P(\{1\}) = \frac{1}{4} \neq P(A_1)P(A_2)P(A_3) = \frac{1}{8}$.

4.13 Random Variables

Example: Three independent coin tosses. $P(x_1, x_2, x_3) = \frac{1}{8}$. The possible outcomes are: (H,H,H), (H,H,T), (H,T,H), (H,T,T), (T,H,H), (T,H,T), (T,T,H), (T,T,T).

For $w \in \Omega$, define $f(w)$ as the number of heads in W. eg. $f(H, T, H) = 2$, $f(T, T, T) = 0$. Or use the notation, $X(w)$ is the number of heads in W. X is called a *random variable.* $X : \Omega \to \Re$. Random variables are functions from Ω to $\Re$ or some subset of $\Re$. For $A \subseteq \Re$, let $X^{-1}(A) = \{W : x(w) \in A\}$.

Using the previous example, $x^{-1}(A) = \{(H, H, H)\}$. $P(x^{-1}(A)) = P(W : x(w) \in A) = P(x \in A)$. So, $P(x = 0) = P(\{W : x(w) \in \{0\}\}) = (T, T, T) = \frac{1}{8}$. $P(x = 1) = P(x \in \{1\}) = (H, T, T), (T, H, T), (T, T, H) = \frac{3}{8}$, and so on. $P(0 \leq x \leq 2) = P(\{W : 0 \leq x(w) \leq 2\}) = P(x = 0) + P(x = 1) + P(x = 2) = \frac{7}{8}$.

4.14 Discrete Random Variables

Example: Three coin tosses. X is the number of heads. Then, $X \in \{0, 1, 2, 3, 4\}$. That is called the *range.* $X(H, T, H) = 2$. For *discrete random variables,* the range is finite and countable. The probability is specified as $P(X = a_i) = x_i$. We must satisfy the following conditions,

1. $\sum P(x = a_i) = 1$.
2. $0 \leq P(x = a_i) \leq 1$.

$P(x = a_i) = x_i$ is called a *probability mass function(pmf).*

Example: Let N be the number of times you must toss a coin to get a 'heads.' $N \in \{1, 2, 3, ...\}$. $P(N = 1) = \frac{1}{2}$, $P(N = 2) = \frac{1}{4}$, $P(N = 3) = \frac{1}{8}$, ... $P(N = k) = \left(\frac{1}{2}\right)^{k-1}\frac{1}{2}$.

$$\sum_{k=1}^{\infty}\left(\frac{1}{2}\right)^{k-1}\frac{1}{2} = \frac{1}{2}\left(1 + \frac{1}{2} + \left(\frac{1}{2}\right)^2 + \cdots\right) = \frac{\frac{1}{2}}{1 - \frac{1}{2}} = 1.$$

4.15 Bernoulli Random Variable

$X \in \{0,1\}$. $P(X=1)=p$, $P(X=0)=1-p$. $X \sim \mathit{Bernoulli}(p)$.

4.16 Distributions

4.16.1 Geometric Distribution

Example: Toss a $p-$biased coin until the first head appears. Let X be the number of tosses required. H_n is 'heads on the n-th toss.' T_n is 'tails on the n-th toss.' $P(X=1)=P(H)=p$. $P(X=0)=P(T_1\cap H_2)=P(T_1)P(H_2)=(1-p)p$.... $P(X=k)=P(T_1\cap\cdots\cap T_{k-1}\cap H_k)=P(T_1)P(T_2)\cdots P(T_{k-1})P(H_k)=(1-p)^{k-1}p$. $X\sim \mathit{geometric}(p)$.

$P(X\text{is odd})=P(x\in\{1,3,5,...\})=P(X=1)+P(X=3)+\cdots$.

$P(X>k)=P(x\in\{k+1,k+2,...\})=P(X=k+1)+P(X=k+2)+\cdots=(1-p)^kp+(1-p)^{k+1}p+\cdots=(1-p)^kp[1+(1-p)+(1-p)^2+\cdots]=(1-p)^kp\frac{1}{1-(1-p)}=(1-p)^k$.

$P(x\in A|x\in B):$

$$P(x>k+n|x>k)=P(x\in\{k+n,k+n+1,...\}|x\in\{k+1,k+2,...\})=$$

$$\frac{P(\{k+n,k+n+1,...\}\cap\{k+1,k+2,...\})}{P(x\in\{k+1,k+2,...\})}=$$

$$\frac{P(x\in\{k+n+1,k+n+2,...\})}{P(x\in\{k+1,k+2,...\})}=\frac{P(x>k+n)}{P(x>k)}=\frac{(1-p)^{k+n}}{(1-p)^k}=(1-p)^k=P(X>n).$$

This is known as the memoryless property of the geometric distribution.

Example: A computer system. $P(\text{system down on a particular day})=0.02$. What is $P(\text{system is trouble free for a month})$? If X is the number of days until the first break down. Then, $X\sim \mathit{Geometric}(0.02)$. $P(X>30)=(1-p)^{30}=(1-0.02)^{30}$.

4.16.2 Binomial Distribution

Example: Three coin tosses. Ω is the same as before. Let A be the number of heads. $P(X=0)=(1-p)^3=\begin{pmatrix}3\\0\end{pmatrix}$. $P(X=1)=\begin{pmatrix}3\\1\end{pmatrix}=p(1-p)^2+p(1-p)^2+p(1-p)^2$. $P(X=2)=3(p^2(1-p))=\begin{pmatrix}3\\2\end{pmatrix}$, etc.

Example: n processor parallel machine. $P(\text{failure})=q$ for each processor. What is $P(\text{less than 3 failures})$? Let X be the number of failed processors. $X\sim \mathit{Binomial}(n,q)$.

$$P(X=k)=\begin{pmatrix}n\\k\end{pmatrix}q^k(1-q)^{n-k}.$$

$$P(\text{less than 3 failures})=P(X<3)=$$

$$P(X=0)+P(X=1)+P(X=2).$$

Example: Suppose there are 6 packs of cards. Draw a card from each deck. What is $P(\text{at least 3 are spades})$? $n=6$. $X\sim \mathit{Binomial}(6,\frac{13}{52})$.

4.16.3 Discrete Uniform Distribution

$X \in \{a_1, ..., a_n\}$. $P(X = a_i) = \frac{1}{n}$.

Example: Die throw. $X \in \{1, 2, 3, 4, 5, 6\}$. $P(X = i) = \frac{1}{6}$.

Other important discrete distributions:

1. Hypergeometric.
2. Negative Binomial(Pascal).
3. Poisson.

4.16.4 Cumulative Distribution Function

May be called distribution functions in other text books. Abbreviated cdf.

$$F(y) = P(X \leq y).$$

Note the following:

1. The cdf is a function of y.
2. It is defined for all y.
3. F is right continuous.
4. $0 \leq F(y) \leq 1$.

Example: Suppose X has the pmf,

$$P(X = 0) = \frac{1}{8},\ P(X = 1) = \frac{3}{8},\ P(X = 2) = \frac{3}{8},\ P(X = 3) = \frac{1}{8}.$$

Then,

$$P(X < 0) = 0,\ P(X \leq 0) = \frac{1}{8},\ P(X \leq 1) = P(X \leq 0) + P(x \leq 1) = \frac{1}{8} + \frac{3}{8} = \frac{4}{8},$$

$$P(X \leq 2) = P(X \leq 1) + P(X = 2) = \frac{4}{8} + \frac{3}{8} = \frac{7}{8},\ P(X \leq 3) = 1,\ P(X \leq 4) = 1.$$

In general, for any pmf $P(X = a_i) = \alpha_i$, $F(y) = P(X \leq y) = \sum_{a_i \leq y} P(X = a_i)$. Note that given a Cumulative distribution function $F(y)$, we can recover the pmf, $P(X = a_i) = \sum_{a_k \leq a_i} P(X = a_i) - \sum_{a_k \leq a_{i-1}} P(X = a_k) = F(a_i) - F(a_{i-1})$.

Example: When X has the pmf:

$$P(X = 0) = \frac{1}{8},\ P(X = 1) = \frac{3}{8},\ P(X = 2) = \frac{3}{8},\ P(X = 3) = \frac{1}{8}.$$

Then, $P(X = 2) = F(2) - F(1) = \frac{7}{8} - \frac{4}{8} = \frac{3}{8}$. So, cdf's and pmf's are both means of 'encoding' a probability measure.

4.16.5 Continuous Random Variables

For a discrete random variable X, the cdf is a step function. Why? Because, the cdf F 'jumps' at the very values the random variable takes on. For continuous random variables, the range is real-valued(uncountable). In this case, F is often continuous, even differentiable. For continuous random variables, we are interested in intervals, $X \in [a, b]$, the set of all reals between a and b. Now,

$$P(X \in [a, b]) = P(X \in (-\infty, b]) - P(X \in (-\infty, a]) = P(X \leq b) - P(X \leq a) = F(b) - F(a).$$

where F is the cdf. So, given the cdf, one can compute $P(X \in [a, b])$. Next, if F is differentiable, then there exists a function f such that,

1. $F(b) - F(a) = \int_a^b f(x)\, dx$.
2. $F'(x) = f(x)$.

Thus,

$$P(X \in [a, b]) = \int_a^b f(x)\, dx.$$

$f(x)$ is called the *probability density function(pdf).* Note:

1. For a cdf $F(y)$,
   (a) $F(y)$ is an increasing function, $y_1 \geq y_2, F(y_1) \geq F(y_2)$.
   (b) $F(y) \to 1$ as $y \to \infty$.
   (c) $F(y) \to 0$ as $y \to -\infty$.
2. $P(X = a) = 0$ for an continuous random variable X and where a is a point of continuity in $F(y)$. We will mostly deal with differentiable functions $F(y)$. So, $P(X = a) = 0$ will always be true for every a.
3. $P(X \leq a) = P(X < a) + P(X = a) = P(X < a) + 0 = P(X < a)$. So we do not need to distinguish between less-than and less-than-and-equal.
4. $\int_{-\infty}^{\infty} f(x)\, dx = 1$.
5. $\int_a^b f(x)\, dx = P(X \in [a, b])$ is the area under the curve $f(x)$ in the interval $[a, b]$.
6. $f(x)$ is not a probability. It is only a device used in computing probabilities.
7. $F(y) = \int_{-\infty}^{\infty} f(x)\, dx$.

Example: Suppose X has the pdf,

$$f(x) = \begin{cases} \frac{3}{8}(4x - 2x^2), & \text{if } 0 < x < 2. \\ 0, & \text{otherwise.} \end{cases}$$

$$F(y) = \int_{-\infty}^{y} f(x)\, dx = \int_0^y \frac{3}{8}(4x - 2x^2)\, dx = \frac{3}{8}\left[\frac{4x^2}{2} - \frac{2x^3}{3}\right]_0^y = \frac{3y^2}{4} - \frac{y^3}{4}, 0 < y < 2.$$

So,

$$F(y) = \begin{cases} 0, & \text{if } y \leq 0. \\ \frac{3y^2}{4} - \frac{y^3}{4}, & \text{if } 0 < y < 2 \\ 1, & \text{if } y \geq 2. \end{cases}$$

One might compute $P(X < 1)$ as follows:

$$P(X < 1) = P(X \in (-\infty, 1]) = \int_{-\infty}^{1} f(x)\,dx = \int_{0}^{1} \frac{3}{8}(4x - 2x^2)\,dx = \frac{1}{2}.$$

Alternatively, since we have computed $F(y)$,

$$P(X < 1) = F(1) = \frac{3}{4} - \frac{1}{4} = \frac{1}{2}.$$

Example: The time to breakdown in hours of a computer system is a continuous random variable with density,

$$f(x) = \begin{cases} 100e^{-100x}, & x \geq 0. \\ 0, & x < 0. \end{cases}$$

What is the probability that a breakdown occurs before 100 hours? Let X be the lifetime of the system. Then, X has the pdf $f(x)$. We want $P(X < 100)$.

$$P(X < 100) = \int_{-\infty}^{100} f(x)\,dx = \int_{0}^{100} 100e^{-100x}\,dx = 100\left[\frac{e^{-100x}}{-100}\right]_0^{100} = 1 - e^{-100^2}.$$

4.16.6 Continuous Uniform Distribution

$X \sim U(\alpha, \beta)$ if the pdf of X is

$$f(x) = \begin{cases} \frac{1}{\beta-\alpha}, & \alpha < x < \beta. \\ 0, & \text{otherwise.} \end{cases}$$

Then,

$$F(y) = \begin{cases} 0, & y \leq \alpha. \\ \frac{y-\alpha}{\beta-\alpha}, & \alpha < y < \beta. \\ 1, & \text{otherwise.} \end{cases}$$

Example: Buses arrive to a bus stop at 7, 7:15, 7:30, 7:45, 8:00 am. You arrive at the bus stop sometime(uniformly) between 7 and 7:30. What is the probability that you will wait less than 5 minutes. Let X be the time of your arrival between 7 and 7:30. Then, we are given $X \sim U(0, 30)$.

$$f(x) = \begin{cases} 0, & x < 0. \\ \frac{1}{30-0}, & 0 < x < 30. \\ 1, & x > 30. \end{cases}$$

$$P(\{10 < x < 15\} \cup \{25 < x < 30\}) = \int_{10}^{15} f(x)\,dx + \int_{25}^{30} f(x)\,dx.$$

4.16.7 Normal Distribution

$X \sim N(\mu, \sigma^2)$ if the density function is

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}.$$

$$F(y) = \int_{-\infty}^{y} f(x)\,dx.$$

4.16.8 Exponential Distribution

$X \sim Exp(\lambda)$.

$$f(x) = \begin{cases} \lambda e^{-\lambda x}, & x \geq 0. \\ 0, & x < 0. \end{cases}$$

$$F(y) = \int_{-\infty}^{y} f(x)\,dx = \int_{0}^{y} \lambda e^{-\lambda x}\,dx = 1 - e^{-\lambda y} = P(x \leq Y).$$

$$P(x > s+u | x > s) = \frac{P(\{x > s+u\} \cap \{x > s\})}{P(\{x > s\})} = \frac{P(x > s+u)}{P(x > s)} = \frac{P(x \in (s+u, \infty))}{P(x \in (s, \infty))} =$$

$$\frac{\int_{s+u}^{\infty} f(x)\,dx}{\int_{s}^{\infty} f(x)\,dx} = \frac{e^{-\lambda(s+u)}}{e^{-\lambda s}} = e^{-\lambda u} = P(X > u).$$

Recall that this was called the memoryless property.

Example: X is the lifetime of a light bulb. $X \sim Exp(\lambda)$.

$$P(x > 3+1 | x > 3) = P(x > 1) =$$

$$P(x > 300+1 | x > 300) = P(x > 1).$$

4.16.9 Other Continuous Distributions

Gamma, Beta, Cauchy, Chi-square, Weibull, Student.

4.17 Functions of Random Variables

X is a random variable. $g : \Re \to \Re$. Then, $y = g(x)$ is a random variable. $X : \Omega \to \Re$.

Example: $X \sim U(0,2), g(x) = x^2$.

$$f_x(x) = \begin{cases} 0, & x \leq 0. \\ \frac{1}{2-0}, & 0 < x < 2. \\ 0, & x \geq 2. \end{cases}$$

$$F_x(x) = \begin{cases} 0, & x \leq 0. \\ \frac{y}{2-0}, & 0 \leq x \leq 2. \\ 1, & \text{otherwise} \end{cases}$$

Let $z = g(x) = x^2$, $F_z(y)$ is a distribution function of $z = P(Z \leq y) =$

$$P(x^2 \leq y) = P(-\sqrt{y} < x < \sqrt{y}) = P(0 < x < \sqrt{y}) = P(x \leq \sqrt{y}) = F_x(\sqrt{y}), 0 < \sqrt{y} < 2.$$

So,

$$F_z(y) = \begin{cases} 0, & \sqrt{y} < 0. \\ \frac{\sqrt{y}}{2-0}, & 0 \leq \sqrt{y} < 2. \\ 1, & \sqrt{y} \geq 2. \end{cases}$$

The probability density function is,

$$f_z(x) = \begin{cases} 0, & x < 0. \\ \frac{1}{4\sqrt{x}}, & 0 < x < 4. \\ 0, & x \geq 4. \end{cases}$$

Example: X is the number of heads in three coin flips. $P(X=0)=\frac{1}{8}, P(X=1)=\frac{3}{8}, P(X=2)=\frac{3}{8}, P(X=3)=\frac{1}{8}$.

$$y=\frac{1}{3x+5}.$$

$$y\in\left\{\frac{1}{3(0)+5},\frac{1}{3(1)+5},\frac{1}{3(2)+5},\frac{1}{3(3)+5}\right\}.$$

$$P(Y=\frac{1}{3(2)+5}=P(x=2).$$

When two values of x give one value of y, then add to obtain the probability.

A discrete event looks like $x\in\{a_1,a_2,...\}$ $P(x=a_i), i=1,2,3,...,n$. $F(y)=P(x\le y)$. The pmf is $f(x)$. $P(a\le x\le b)=\int_a^b f(x)\,dx$. $F(y)=P(x\le y)=\int_{-\infty}^y f(x)\,dx$.

4.18 Joint Distributions

Example: Three coin tosses. X is the number of heads. Define y as:

$$y=\begin{cases}1, & \text{if \# heads} > \text{\# tails.}\\ 0, & \text{otherwise.}\end{cases}$$

$w\in\Omega$	$x(w)$	$y(w)$	$P(w)$
HHH	3	1	$\frac{1}{8}$
HHT	2	1	$\frac{1}{8}$
HTH	2	1	$\frac{1}{8}$
HTT	1	0	$\frac{1}{8}$
THH	2	1	$\frac{1}{8}$
THT	1	0	$\frac{1}{8}$
TTH	1	0	$\frac{1}{8}$
TTT	0	0	$\frac{1}{8}$

The ranges are $R_x=\{0,1,2,3\}$ and $R_y=\{0,1\}$. The range of (x,y) is $R_x\times R_y=\{(x,y):x\in R_x; v\in R_y\}=\{(0,0),(0,1),(1,0),(1,1),(2,0),(2,1),(3,0),(3,1)\}$. The joint pmf is

$$P(x=i,y=j),(i,j)\in R_{xy}=P(\{w\in\Omega:x(w)=i\text{ and }y(w)=j\}).$$

For example, $P(x=3,y=1)=P(\{W:x(w)=3,y(w)=1\})=P(\{(HHH)\}=\frac{1}{8}$. $P(x=2,y=1)=P(\{(HHT),(HTH),(THH)\})=\frac{3}{8}$.

x/y	0	1
0	$\frac{1}{8}$	0
1	$\frac{3}{8}$	0
2	0	$\frac{3}{8}$
3	0	$\frac{1}{8}$

$$\sum_{(i,j)\in R_{xy}} P(x=i,y=j)=1.$$

4.19 Marginal Distributions

The marginal pmf of X is defined as $P_x(x = i), i \in R_x$.

$$\sum_{j \in R_y} P(x = i, y = j).$$

For example,

$$P(x = 0) = \sum_{j \in R_y} P(x = 0, y = i) = P(x = 0, y = 0) + P(x = 0, y = 1) = \frac{1}{8} + 0 = \frac{1}{8}.$$

$$P(x = y) = P(x = i, y = j; i = j) = P(x = 0, y = 0) + P(x = 1, y = 1) = \frac{1}{8} + 0 = \frac{1}{8}.$$

4.20 Independence

Random variables x and y are independent if for every $A \subseteq R_x, B \subseteq R_y, P(x \in A, y \in B) = P_x(x \in A)P_y(y \in B)$.

Example: Coin toss and die throw.

$$x = \begin{cases} 1, & \text{if heads.} \\ 0, & \text{otherwise.} \end{cases}$$

Y is the number on the die. Assume independence. $P(x = 0) = \frac{1}{2}$. $P(x = 1) = \frac{1}{2}$. $P(y = k) = \frac{1}{6}, k = 1, 2, 3, 4, 5, 6$. $P(x = i, y = j) = P(x = i)P(y = j)$. eg. $P(x = 0, y = 1) = \frac{1}{2}\left(\frac{1}{6}\right) = \frac{1}{12}$.

4.21 Conditional Probability

$$P(x \in A | y \in B) = \frac{P(x \in A, y \in B)}{P(y \in B)}.$$

Example: A coin toss and die throw(same as before).

$$P(x = 1 | y \in \{1, 2\}) = \frac{P(x \in \{1\} | y \in \{1, 2\})}{P(y \in \{1, 2\})} = \frac{P(x \in \{1\})P(y \in \{1, 2\})}{P(y \in \{1, 2\})} = P(x \in \{1\}) = \frac{1}{2}.$$

Example: $x \in \{0, 1\}$, $y \in \{0, 1\}$.

x/y	0	1
0	0.4	0.2
1	0.1	0.3

$$P(x = 0 | y = 1) = \frac{P(x = 0, y = 1)}{P(y = 1)} = \frac{0.2}{0.2 + 0.3} = \frac{2}{5}.$$

Alternate notation is $P_{y=1}(x = 0)$.

$$P(x = 1 | y = 1) = \frac{P(x = 1, y = 1)}{p(y = 1)} = \frac{0.3}{0.5} = \frac{3}{5}.$$

Alternate notation is $P_{y=1}(x = 1)$.

Generally, $x \in R_x = \{a_1, a_2, ...\}$, and $y \in R_y = \{b_1, b_2, ...\}$. The conditional pmf of x is given by $y = b_k$, $P(x = a_1 | y = b_k)$, $P(x = a_2 | y = b_k)$, $P(x = a_3 | y = b_k)$, ...

4.22 Distribution Functions

1. Joint distribution function $P(x \leq a_i, y \leq b_j)$.
2. Conditional distribution function $P(x \leq a | y \leq b)$.

4.23 Homework and Answers

1. An urn contains 3 red balls, 2 blue balls and a green ball. Two balls are drawn in succession without replacement. Let X denote the number of red balls among those drawn and define Y as follows:

$$Y = \begin{cases} 1, & \text{if first ball is green.} \\ 0, & \text{otherwise.} \end{cases}$$

Write down the sample space and the values of the random variables X and Y for each element of the sample space. Identify all elements of the sample space for which $X = 1$. What are the probability mass functions of X and Y? Compute the distribution functions of X and Y. Compute $P(X = 2|X > 0)$. $\Omega = \{(R,R),(R,B),(R,G),(B,B),(B,R),(G,R),(G,B),(B,G)\}$.

$$P(\{(R,R)\}) = \frac{3}{6}\left(\frac{2}{5}\right) = \frac{6}{30},\ P(\{(R,B)\}) = \frac{3}{6}\left(\frac{2}{5}\right) = \frac{6}{30},\ P(\{(R,G)\}) = \frac{3}{6}\left(\frac{1}{5}\right) = \frac{3}{30},$$

$$P(\{(B,B)\}) = \frac{2}{6}\left(\frac{1}{5}\right) = \frac{2}{30},\ P(\{(B,R)\}) = \frac{2}{6}\left(\frac{3}{5}\right) = \frac{6}{30},\ P(\{(G,R)\}) = \frac{1}{6}\left(\frac{3}{5}\right) = \frac{3}{30}.$$

$$P(\{(G,B)\}) = \frac{1}{6}\left(\frac{2}{5}\right) = \frac{2}{30},\ P(\{(B,G)\}) = \frac{2}{6}\left(\frac{1}{5}\right) = \frac{2}{30}.$$

X is the number of red balls. $x \in \{0,1,2\}$. At $x = 1$, the elements of the sample space are $\{(R,B),(R,G),(B,R),(G,R)\}$. The probability mass functions for x are:

$$P(x = 0) = \frac{2}{30} + \frac{2}{30} + \frac{2}{30} = \frac{6}{30}.$$

$$P(x = 1) = \frac{6}{30} + \frac{3}{30} + \frac{6}{30} + \frac{3}{30} = \frac{18}{30}.$$

$$P(x = 2) = \frac{6}{30}.$$

The probability mass functions for y are:

$$P(y = 0) = \frac{6}{30} + \frac{6}{30} + \frac{3}{30} + \frac{2}{30} + \frac{6}{30} + \frac{2}{30} = \frac{25}{30}.$$

$$P(y = 1) = \frac{3}{30} + \frac{2}{30} = \frac{5}{30}.$$

The distribution functions of x are:

$$P(x \leq 0) = P(x = 0) = \frac{6}{30}.$$

$$P(x \leq 1) = P(x \leq 0) + P(x = 1) = \frac{6}{3} + \frac{18}{30} = \frac{24}{30}.$$

$$P(x \leq 2) = P(x \leq 1) + P(x = 2) = \frac{24}{30} + \frac{6}{30} = 1.$$

The distribution functions of y are:

$$P(y \leq 0) = P(y = 0) = \frac{25}{30}.$$

$$P(y \le 1) = P(y \le 0) + P(y = 1) = \frac{25}{30} + \frac{5}{30} = 1.$$

$$P(x = 2|x > 0) = \frac{P((x = 2) \cap (x > 0))}{P(x > 0)} = \frac{P(\{(R, R)\} \cap \{(R, B), (R, G), (B, R), (G, R), (R, R)\})}{P(\{(R, R), (R, B), (R, G), (B, R), (G, R)\})} =$$

$$\frac{P(\{(R, R)\})}{P(\{(R, R), (R, B), (R, G), (B, R), (G, R)\})} = \frac{\frac{6}{30}}{\frac{6}{30} + \frac{6}{30} + \frac{3}{30} + \frac{6}{30} + \frac{3}{30}} = \frac{6}{24} = \frac{1}{4}.$$

2. Students at W& M bring their diskettes in to a Virus Testing Center in Jones Hall to have them checked for viruses. The probability of a diskette containing a virus is 0.05 independent of other diskettes. Identify appropriate Bernoulli, Binomial and Geometric random variables in this sequence of experiments. Use your definitions to compute:

   (a) The probability that at least 2 among the first 10 tested contain a virus.

   $X \sim Bernoulli(0.05)$. Let X be the number of diskettes tested until one contains a virus. $x \in \{0, 1\}$. $P(x = 1) = 0.05 = p$. $P(x = 0) = 0.95 = q$. Now, let X be the number of tests performed until a virus occurs. $X \sim Geometric(0.05)$. v_n is 'virus on the n-th disk.' F_n is 'no virus on the n-th disk.'

   $$P(x = 1) = P(v_1) = p = 0.05.$$

   $$P(x = 2) = P(F_1 \cap v_2) = P(F_1)P(v_2) = (1 - p)p = (0.95)(0.05).$$

   $$P(x = 3) = P(F_1 \cap F_2 \cap v_3) = P(F_1)P(F_2)P(v_3) = (1 - p)^2 p = (0.95)^2(0.05).$$

   $$P(x = k) = P(F_1 \cap F_2 \cap \cdots \cap F_{k-1} \cap v_k) = (1 - p)^{k-1} p = (0.95)^{k-1}(0.05).$$

   Now, let X be the number of diskettes with a virus. $X \sim Binomial(n, 0.05)$. $x \in \{0, 1, 2, ..., n\}$. $P(x = k) = \begin{pmatrix} \text{n} \\ \text{k} \end{pmatrix} q^k (1 - q)^{n-k}$.

   For part (a), use the binomial distribution.

   $$P(x \ge 2) = 1 - p(x = 1) - P(x = 0) = 1 - \begin{pmatrix} 10 \\ 1 \end{pmatrix} (0.05)^1 (0.95)^{10-1} - \begin{pmatrix} 10 \\ 0 \end{pmatrix} (0.05)^0 (0.95)^{10}.$$

   (b) The probability that the 3-rd diskette to be tested is the first to contain a virus.

   Use the geometric distribution.

   $$P(\text{3-rd disk contains virus}) = P(x = 3) = (1 - 0.05)^{3-1}(0.05) \approx 0.045.$$

3. Suppose Z is Geometrically distributed with parameter p. What is the probability that Z is odd(i.e. that $Z's$ value is an odd number)? What is the probability that Z is even? Obtain expressions in terms of p.

4. A system has five identical components. The lifetime of each component in years is a random variable with a density given by

   $$f(x) = \begin{cases} 0, & x \le 5. \\ \frac{c}{x^2}, & x > 5. \end{cases}$$

   What is the value of c that makes f a probability density function? What is the probability that exactly two components will have to be replaced before 10 years? Assume independence between components.

The probability that one component will breakdown before 10 years is

$$\int_{-\infty}^{10} f(x)\,dx = \int_{-\infty}^{5} f(x)\,dx + \int_{5}^{10} f(x)\,dx = 0 + \int_{5}^{10} \frac{5}{x^2}\,dx = -\frac{5}{x}\bigg|_{5}^{10} = -\frac{5}{10} + \frac{5}{5} = \frac{1}{2}.$$

Let Y be the number of components. Each component is a Bernoulli trial.

$P(2 \text{ components will break down}) =$

$$P(y=2) = \left(\begin{array}{c} 5 \\ 2 \end{array}\right)\left(\frac{1}{2}\right)^2\left(\frac{1}{2}\right)^{5-2} = \frac{5!}{2!(5-2)!}\left(\frac{1}{2}\right)^2\left(\frac{1}{2}\right)^3 = \frac{10}{32} = 0.31.$$

5. Y is a random variable with the following density function

$$f(x) = \begin{cases} \frac{1}{2}\lambda e^{-\lambda x}, & x > 0. \\ \frac{1}{2}\lambda e^{\lambda x}, & x \le 0. \end{cases}$$

Find the distribution function of Y.

$$F(y) = \int_0^y \frac{1}{2}\lambda e^{-\lambda x}\,dx + \int_{-\infty}^{0} \frac{1}{2}\lambda e^{\lambda x}.$$

4.24 Convolution(Discrete Case)

$h(x, y) = x + y$.

Example:

x/y	3	4
1	0.2	0.3
2	0.1	0.4

$R_x = \{1, 2\}$. $R_y = \{3, 4\}$. Let $z = x + y$. $R_z = \{4, 5, 6\}$.

$$P(z=4) = \sum_{(i,j)=i+j=4} P(x=i, y=j) = P(x=1, y=3) = 0.2.$$

$$P(z=5) = P(x=2, y=3) + P(x=1, y=4) = 0.1 + 0.3 = 0.4.$$

$$P(z=6) = P(x=2, y=4) = 0.4.$$

Example: $X \sim Poisson(\lambda_1)$, $Y \sim Poisson(\lambda_2)$. $z = x + y$. X has the pmf:

$$P(x=k) = \frac{e^{-\lambda_1}\lambda_1^k}{k!}, k = 0, 1, 2, ...$$

Y has the pmf:

$$P(y=k) = \frac{e^{-\lambda_2}\lambda_2^k}{k!}, k = 0, 1, 2, ...$$

$R_x = \{0, 1, 2, ...\}$

$R_y = \{0, 1, 2, ...\}$

$R_z = \{0, 1, 2, ...\}$

$$P(z=k) = \sum_{(i,j)=i+j=k} P(x=i, y=j) = \sum_i P(x=i, y=k-i) = \sum_{0\le i\le k} P(x=i)(P(y=k-i) =$$

$$\sum_{i=0}^{k} \frac{e^{-\lambda_1}\lambda_1^i}{k!}\frac{e^{-\lambda_2}\lambda_2^{k-i}}{(k-i)!} = \frac{e^{-\lambda_1}e^{-\lambda_2}}{k!}\sum_{i=1}^{k}\frac{k!}{i!(k-i)!}\lambda_1^i\lambda_2^{k-i} = \frac{e^{-(\lambda_1+\lambda_2)}(\lambda_1+\lambda_2)^k}{k!}.$$

The sum of two Poisson processes is Poisson.

4.25 Convolution(Continuous Case)

x has the pdf, $f_x(x)$. y has the pdf, $f_y(y)$. x and y are independent. $z = x + y$. We want the pdf of Z. $F_z(z)$ is the cdf of Z.

$$P(Z \leq z) = P(x + y \leq z) = \int \int_A f(x,y)\,dx\,dy,$$

where $A = \{(x,y) : x + y \leq z\}$.

$$\int_{-\infty}^{\infty} \int_{-\infty}^{z-y} f_x(x) f_y(y)\,dx\,dy = \int_{-\infty}^{\infty} f_y(y) \left(\int_{-\infty}^{z-y} f_x(x)\,dx \right) dy = \int_{-\infty}^{\infty} f_y(y) F_x(z-y)\,dy.$$

The above equations are called convolutions.

1. $x_i \sim Bernoulli(p)$.

$$y = \sum_{i=1}^{n} x_i = x_1 + x_2 + \cdots + x_n.$$

$$y \sim Binomial(n,p).$$

2. $x_i \sim Poisson(\lambda_i)$.

$$y = \sum_{i=1}^{n} x_i = x_1 + x_2 + \cdots + x_n.$$

$$y \sim Poisson(\lambda_1 + \lambda_2 + \cdots + \lambda_n)$$

3. $x_i \sim N(\mu_i, \sigma_i^2)$.

$$y = \sum_{i=1}^{n} x_i = x_1 + x_2 + \cdots + x_n.$$

$$y \sim N\left(\sum_{i=1}^{n} \mu_i, \sum_{i=1}^{n} \sigma_i^2 \right).$$

4.26 Expectation

4.26.1 Expectation(Discrete Case)

$X \in \{a_1, a_2, ...\}$. $E(x) = \sum_i a_i P(x = a_i)$.

Example: $X \sim Bernoulli(p)$. $x \in \{0,1\}$.

$$E(x) = 0P(x=0) + 1P(x=1) = p.$$

Example: $X \sim Geometric(p)$. $P(x=k) = (1-p)^{k-1}p$.

$$E(x) = \sum_{k=0}^{\infty} kP(x=k) = \sum_{k=1}^{\infty} k(1-p)^{k-1}p.$$

Let $q = 1 - p$, then

$$E(x) = p\sum_{k=1}^{\infty} kq^{k-1} = p\sum_{k=1}^{\infty} \frac{\partial q^k}{\partial q} = p\frac{\partial}{\partial q}\left(\sum_{k=1}^{\infty} q^k \right) = p\frac{\partial}{\partial q}\left(\frac{1}{1-q} \right) = \frac{p}{(1-q)^2} = \frac{p}{p^2} = \frac{1}{p}.$$

Example: $X \sim Poisson$.

$x \in \{0, 1, 2, ...\}$.

$E(x) = \sum_{k=0}^{\infty} kP(x = k) = \sum_{k=0}^{\infty} \frac{kE^{-\lambda}\lambda^k}{k!} = 0 + \frac{e^{-\lambda}\lambda^1}{1!} + \frac{2e^{-\lambda}\lambda^2}{2!} + \frac{3e^{-\lambda}\lambda^3}{3!} + \cdots =$

$e^{0\lambda}\lambda \left[1 + \lambda + \frac{\lambda^2}{2!} + \frac{\lambda^3}{3!} + \cdots\right] = e^{-\lambda}\lambda e^{\lambda} = \lambda.$

4.26.2 Expectation(Continuous Case)

x has the pdf $f(x)$.

$$E(x) = \int_{-\infty}^{\infty} xf(x)\,dx.$$

Example: $X \sim U(\alpha, \beta)$.

$$f(x) = \begin{cases} \frac{1}{\beta-\alpha}, & \alpha < x < \beta. \\ 0, & \text{otherwise.} \end{cases}$$

$$E(x) = \int_{-\infty}^{\infty} xf(x)\,dx = \int_{\alpha}^{\beta} \frac{x}{\beta-\alpha}\,dx = \frac{1}{\beta-\alpha}\left[\frac{x^2}{2}\right]_{\alpha}^{\beta} = \frac{1}{\beta-\alpha}\frac{1}{2}(\beta^2 - \alpha^2) = \frac{\beta+\alpha}{2}.$$

Example: $X \sim Exp(\lambda)$.

$f(x) = \lambda e^{-\lambda x}, x \geq 0.$

$$E(x) = \int_{-\infty}^{\infty} xf(x)\,dx = \int_{-\infty}^{\infty} x\lambda e^{-\lambda x}\,dx = \frac{1}{\lambda}.$$

4.26.3 Expectation of a Function

$y = g(x)$. We are given the distribution of x. Suppose $y = x^2$, $R_x \in \{0, 1, 2\}$, $R_y \in \{0, 1, 4\}$.

E(y): $P(y = 0) = \frac{1}{4}$,

$P(y = 1) = \frac{1}{2}$,

$P(y = 2) = \frac{1}{4}$.

$$E(y) = \sum_{k=0,1,4} kP(y = k) = (0)\frac{1}{4} + (1)\frac{1}{2} + (4)\frac{1}{4} = \frac{3}{2}.$$

Or, alternatively,

$$E(y) = E(g(x)) = \sum_{k \in R_y} g(k)P(x = k) = (0^2)\frac{1}{2} + (1^2)\frac{1}{2} + (2^2)\frac{1}{4} = \frac{3}{2}.$$

For the continuous case.

$$E(g(x)) = \int_{-\infty}^{\infty} g(x)f(x)\,dx,$$

where $f(x)$ is the pmf of x.

Example: $X \sim U(0, 1)$. $g(x) = e^x$.

$$E(g(x)) = \int_{-\infty}^{\infty} g(x)f(x)\,dx = \int_0^1 e^x 1\,dx = e - 1.$$

4.26.4 Properties of Expectation

1. $E(ax+b) = aE(x)+b$.
   Proof:
$$E(ax+b) = \sum_k (ax+b)P(x=k) = \sum_k axP(x=k) + b\sum_k P(x=k) = aE(x)+b.$$

2. $E(x+y) = E(x)+E(y)$.
   Proof:
$$E(x+y) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(x+y)f(x,y)\,dx\,dy = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}xf(x,y)\,dx\,dy + \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}yf(x,y)\,dx\,dy =$$
$$\int_{-\infty}^{\infty}x\int_{-\infty}^{\infty}f(x,y)\,dx\,dy + \int_{-\infty}^{\infty}y\int_{-\infty}^{\infty}f(x,y)\,dx\,dy = \int_{-\infty}^{\infty}xf_y(x)\,dx + \int_{-\infty}^{\infty}yf_x(y)\,dy = E(x)+E(y).$$

3. $E(x_1+\cdots+x_n) = E(x_1)+E(x_2)+\cdots+E(x_n)$.

   Example: $x_i \sim Bernoulli(p), i = 1, 2, 3, \ldots$ Let
$$y_n = \sum_{y=1}^{n} x_i.$$
$$E(y_n) = E\left(\sum_{i=1}^{n} x_i\right) = \sum_{i=1}^{n} E(x_i) = E(x_i) = 0(1-p)+1p = p\sum_{i=1}^{n} p = np.$$
   Thus, Y is Binomially distributed.

4. Infinite sum.
$$E\left(\sum_{i=1}^{\infty} x_i\right) = \sum_{i=1}^{\infty} E(x_i),$$
   where either:
   (a) x_i are non-negative ($P(x_i \geq 0) = 1$).
   (b) $\sum_{i=1}^{\infty} E(|x_i|) < \infty$.

5. Suppose x is 1) non-negative and 2) integer-valued. Then,
$$E(x) = \sum_{i=1}^{\infty} P(x \geq i).$$
   Proof:
$$Y_i = \begin{cases} 1, & \text{if } x \geq i. \\ 0, & \text{if } x < i. \end{cases}$$
   Then,
$$\sum_{i=1}^{\infty} Y_i = \sum_{i=1}^{x} Y_i + \sum_{i=x+1}^{\infty} Y_i = \sum_{i=1}^{x} 1 + \sum_{x+1}^{\infty} 0 = x.$$
$$E(x) = \sum_{i=1}^{\infty} E(Y_i) = \sum_{i=1}^{\infty}(0)P(x<i) + (1)P(x \geq i) = \sum_{i=1}^{\infty} P(x \geq i).$$

Example: A linked list. Element i is accessed with probability α_i. Let Y be the number of links traversed. $R_y = \{1, 2, ..., n\}$. $P(y = k) = \alpha_i$.

$$E(y) = \sum_{k=1}^{n} kP(y = k) = \sum_{k=1}^{n} k\alpha_k \leq \sum_{k=1}^{n} k.$$

Assume a uniform distribution. Then,

$$\sum_{k=1}^{n} \frac{k}{n} = \frac{1}{n}\frac{n(n+1)}{2} = \frac{n+1}{2}.$$

Prove the list should be ordered in the form of decreasing probabilities. Assume that $\alpha_1 \geq \alpha_2 \geq \alpha_3 \geq \cdots \geq \alpha_n$ and let $\bigcirc_1$ be the ordering $1, 2, ..., n$, and $\bigcirc_2$ be any other ordering, $i_1, i_2, ..., i_n$.

$$P_{\bigcirc_2}(y \geq k) = \sum_{j=k}^{n} \alpha_{i_j} = \alpha_{i_k} + \alpha_{i_{k+1}} + \cdots + \alpha_{i_n} \geq \alpha_k + \alpha_{k+1} + \cdots + \alpha_n = P_{\bigcirc_1}(y \geq k).$$

So,

$$P_{\bigcirc_2}(y \geq k) \geq P_{\bigcirc_1}(y \geq k).$$

Then,

$$\sum_{k=1}^{n} P_{\bigcirc_2}(y \geq k) \geq \sum_{k=1}^{n} P_{\bigcirc_1}(y \geq k).$$

Then, $E_{\bigcirc_2}(y) \geq E_{\bigcirc_1}(y)$.

The pdf of a distribution is given by $f(x)$ for a random variable X. The cdf of a random variable is $P(x \int [a, b]) = \int_a^b f(x)\,dx$ for the continuous case. If $A = [a, b]$, then, $P(x \in A) = \int_A f(x)\,dx$. If $A = [a, b] \cup [c, d]$, $\int_A f(x)\,dx = \int_a^b f(x)\,dx + \int_c^d f(x)\,dx$.

4.27 Joint Distributions

Compute a joint density function for $f(x, y)$.

$$P(x \in A, y \in B) = \int_B \int_A f(x, y)\,dx\,dy.$$

Example: The joint pdf of x and y is

$$f(x, y) = \begin{cases} 2e^{-x}e^{-2y}, & \text{if } 0 < x < \infty; 1 < y < \infty. \\ 0, & \text{otherwise.} \end{cases}$$

Then, $\partial F(u, v)$ is a distribution function.

$$F(u, v) = P(x \leq u, y \leq v).$$

$$\int_{x \in u} \int_{y \in v} f(x, y)\,dx\,dy = \int_{-\infty}^{u} \int_{-\infty}^{v} f(x, y)\,dx\,dy = \int_0^u \int_0^v f(x, y)\,dx\,dy = \int_0^u \int_0^v 2e^{-x}e^{-2y}\,dx\,dy =$$

$$\int_0^u -2e^{-x}e^{-2y}\,dy\Big|_0^v = \int_0^u -2e^{-v}e^{-2y} + 2e^{-2y}\,dy = \frac{-2e^{-v}e^{-2y}}{-2} + \frac{2e^{-2y}}{-2}\Big|_0^u = (1 - e^{-v})(1 - e^{-2u}).$$

Example:

$$P(x > 1, y < 1) = \int_{-\infty}^{1} \int_1^{\infty} f(x, y)\,dx\,dy = \int_{-\infty}^{1} \int_1^{\infty} 2e^{-x}e^{-2y}\,dx\,dy = e^{-1}(1 - e^{-2}).$$

Example:

$$P(x < y) = \int\int_A f(x, y)\,dx\,dy.$$

Define $A = \{(x, y) : x < y\}$. Then,

$$\int_{-\infty}^{\infty}\int_{-\infty}^{y} 2e^{-x}e^{-2y}\,dx\,dy.$$

Example:

$$P(x < a) = \int\int_A f(x, y)\,dx\,dy.$$

$A = \{(x, y) : x < a.\}$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x, y)\,dx\,dy.$$

4.28 Marginal Distributions

Suppose x and y have the joint pdf of $f(x, y)$. The marginal pdf of x is

$$f_x(x) = \int_{-\infty}^{\infty} f(x, y)\,dy.$$

The marginal pdf of y is

$$f_y(y) = \int_{-\infty}^{\infty} f(x, y)\,dx.$$

Using the same example, then

$$f_x(x) = \int_{-\infty}^{\infty} 2e^{-x}e^{-2y}\,dy = \frac{2e^{-x}e^{-2y}}{-2}\bigg|_{-\infty}^{\infty} = e^{-x}.$$

And,

$$f_y(y) = \int_{-\infty}^{\infty} 2e^{-x}e^{-2y}\,dx = -2e^{-x}e^{-2y}\bigg|_{-\infty}^{\infty} = 2e^{-2y}.$$

4.29 Independence

$P(x \in A, y \in B) = P(x \in A)P(y \in B)$. An alternative definition is $f(x, y) = f_x(x)f_y(y)$ or $F(u, v) = F_x(u)F_y(v)$.

4.30 Conditional Distributions

For the discrete case, given $Y = y$, $P(x = a_i|Y = y)$. For the continuous case, $f_{x|Y=y}(x) = \frac{f(x,y)}{f_y(y)}$. $P(x \in A|Y = y) = \int_A f_{x|Y=y}(x, y)\,dx$.

Example:

$$f(x,y) = \begin{cases} \frac{e^{-\frac{x}{y}}e^{-y}}{y}, & \text{if } 0 < x < \infty. \\ y, & \text{if } 0 < y < \infty. \\ 0, & \text{otherwise} \end{cases}$$

Find $P(x > 1|Y = y)$.

$$f_y(y) = \int_{-\infty}^{\infty} f(x,y)\,dx = \int_{-\infty}^{\infty} \frac{e^{-\frac{x}{y}}e^{-y}}{y}\,dx = \left.\frac{e^{-\frac{x}{y}}e^{-y}}{y\left(-\frac{1}{y}\right)}\right|_0^{\infty} = \left.-e^{-\frac{x}{y}}e^{-y}\right|_0^{\infty} = e^{-y}.$$

Then,

$$f_{x|Y=y} = \frac{e^{-\frac{y}{x}}e^{-y}}{\frac{y}{e^{-y}}} = \frac{e^{-\frac{x}{y}}}{y}.$$

Then,

$$P(x > 1|Y = y) = \int_1^{\infty} f_{x|Y=y}(x)\,dx = \int_1^{\infty} \frac{e^{-\frac{x}{y}}}{y}\,dx = \frac{1}{y}\left[\frac{e^{-\frac{x}{y}}}{-\frac{1}{y}}\right]_1^{\infty} = e^{-\frac{1}{y}}.$$

For a collection of random variables, $x_1, x_2, ..., x_k$, $P(x_1 = i_1, x_2 = i_2, ..., x_k = i_k)$ is the joint pmf. The joint density function is $P(x_1 \le i_1, x_2 \le i_2, ..., x_k \le i_k)$. R_{x_i} is a range for one variable. $\Re = R_{x_1} \times R_{x_2} \times \cdots \times R_{x_k}$ The conditional function is $f(x_1, x_2, ..., x_k)$, $P(x_1 = i_1, x_2 = i_2 | x_3 = i_3, x_4 = i_4, ..., x_k = i_k)$. $x_1, x_2, ..., x_A$ are independent if for every subgroup $x_1, ..., x_k$, and events $A_1, A_2, ..., A_k$, $P(x_{n_1} \in A_1, x_{n_2} \in A_2, ..., x_{n_k} \in A_k) = P(x_{n_1} \in A_1)P(x_{n_2} \in A_2) \cdots P(x_{n_k} \in A_k)$.

If $x_1, x_2, ..., x_n$ and $y_1, y_2, ..., y_n$ are independent and $h : \Re^n \to \Re$, $g : \Re^n \to \Re$ are functions and $u = h(x_1, x_2, ..., x_n)$, $v = g(y_1, y_2, ..., y_n)$, then u and v are random variables, and u and v are independent.

4.31 Conditional Expectation

Let there be a random number of random variables. Let $x_1, x_2, ...$ be an iid sequence and N be an integer valued random variable. $N \in \{1, 2, 3, ...\}$. Let $z = \sum_{i=1}^{N} x_i$. What is $E(z)$? $E(z) = E(N)\mu$, $\mu = E(x)$; Use $E(x) = \sum_Y E(x|Y = y)P(Y = y)$. So,

$$E(z) = \sum_k E(z|N = k)P(N = k) = \sum_k E\left(\sum_{i=1}^{N} x_i | N = k\right) P(N = k) = \sum_k k\mu P(N = k) =$$

$$\mu \sum_k kP(N = k) = \mu E(N).$$

Example: A linked list. Use the head of the line strategy. Let n be the number of elements in the list. Let y be the access depth for a random variable under the head of the line strategy. α_i is the probability element i is accessed. u_i is the position of element i at time of access. Find $E(y)$.

$$E(y) = \sum_{i=1}^{n} E(Y|\ i \text{ is accessed})\alpha_i = \sum_{i=1}^{n} E(v_i)\alpha_i.$$

Let,

$$w_j = \begin{cases} 1, & \text{if } j \text{ preceeds } i \text{ in the list.} \\ 0, & \text{otherwise.} \end{cases}$$

Then,

$$v_i = 1 + \sum_{j \neq i} w_j.$$

$$E(v_i) = E(1) + \sum_{j \neq i} E(w_j).$$

$$E(w_j) = 0P(w_j = 0) + 1P(w_j = 1) = P(w_j = 1).$$

$$P(j \text{ preceeds } i.) = P(\text{previouse access for } j \text{ or } i \text{ accessed } j.) =$$

$$P(j \text{ is accessed}|j \text{ or } i \text{ is accessed}) = \frac{P(j \text{ is accessed})}{P(j \text{ or } i \text{ is accessed})} = \frac{\alpha_i}{\alpha_i + \alpha_j}.$$

So,

$$E(v_i) = 1 + \sum_{j \neq i} \frac{\alpha_j}{\alpha_i + \alpha_j}.$$

$$E(y) = \sum_{i=1}^{n} \alpha_i E(v_i) = \sum_{i=1}^{n} \alpha_i \left(1 + \sum_{j \neq i} \frac{\alpha_j}{\alpha_i + \alpha_j}\right).$$

Note that,

$$P(x \in A|y \in B) = \frac{P(x \in A, y \in B)}{P(y \in B)}.$$

For three random variables, x_1, x_2, x_3,

$$P(x_3 \in A_3|x_1 \in A_1, x_2 \in A_2) = \frac{P(x_1 \in A_1, x_2 \in A_2, x_3 \in A_3)}{P(x_1 \in A_1, x_2 \in A_2)}.$$

k_1, k_2, k_3	$P(x_1 = k_1, x_2 = k_2, x_3 = k_3)$
(1,2,3)	0.04
(1,3,3)	0.40
(1,2,1)	0.06
(2,1,2)	0.06
(2,1,3)	0.24
(2,3,3)	0.20

$$P(x_3 = 3|x_1 = 1, x_2 = 2) = \frac{P(x_1 = 1, x_2 = 2, x_3 = 3)}{P(x_1 = 1, x_2 = 2)} = \frac{0.04}{0.04 + 0.06}.$$

$$P(x_3 = 3|x_2 = 2) = \frac{P(x_2 = 2, x_3 = 3)}{P(x_2 = 2)} = \frac{0.04}{0.04 + 0.06}.$$

The two above calculations are the same due to the intrinsic nature of the problem.

4.32 Homework and Answers

1. Some entries in the table representing the joint pmf of random variables X and Y are given below:

	0	1	2	
0	0.1	a	b	0.3
1	c	0.1	d	0.2
2	e	f	0.3	g
	0.1	h	0.4	

Fill in the missing entries to make it a joint pmf; explain how you obtained the missing entries[Hint: read Example 6 on page 212 of your textbook. *Do not assume* independence in this problem]. Then answer the following: $1 = 0.3 + 0.2 = g \Rightarrow g = 0.5$. $1 = 0.1 + h + 0.4 \Rightarrow h = 0.5$. $0.1 = 0.1 + c + e \Rightarrow 0 = c + e$. Since $0 \leq c \leq 1$, and $0 \leq e \leq 1$, it must be that $c = e = 0$ for the equation to hold true. $0 + 0.1 + d = 0.2 \Rightarrow d = 0.1$. $0 + f + 0.3 = 0.5 \Rightarrow f = 0.2$. $a + 0.1 + 0.2 = 0.5 \Rightarrow a = 0.2$. $b + 0.1 + 0.3 = 0.4 \Rightarrow b = 0$. So, the joint pmf of x and y is:

	0	1	2	
0	0.1	0.2	0	0.3
1	0	0.1	0.1	0.2
2	0	0.2	0.3	0.5
	0.1	0.5	0.4	

(a) What are the marginal pmf's and cdf's of X and Y? Compute $E(X)$ and $E(Y)$. Are X and Y independent? The marginal pmf's of x are:

$$P_x(x = 0) = P(x = 0, y = 0) + P(x = 0, y = 1) + P(x = 0, y = 2) = 0.1 + 0.2 + 0 = 0.3.$$

$$P_x(x = 1) = P(x = 1, y = 0) + P(x = 1, y = 1) + Px = 1, y = 2) = 0 + 0.1 + 0.1 = 0.2.$$

$$P_x(x = 2) = P(x = 2, y = 0) + P(x = 2, y = 1) + P(x = 2, y = 2) = 0 + 0.2 + 0.3 = 0.5.$$

The marginal pmf's of y are:

$$P_y(y = 0) = P(x = 0, y = 0) + P(x = 1, y = 0) + P(x = 2, y = 0) = 0.1 + 0 + 0 = 0.1.$$

$$P_y(y = 1) = P(x = 0, y = 1) + P(x = 1, y = 1) + P(x = 2, y = 1) = 0.2 + 0.1 + 0.2 = 0.5.$$

$$P_y(y = 2) = P(x = 0, y = 2) + P(x = 1, y = 2) + P(x = 2, y = 2) = 0 + 0.1 + 0.3 = 0.4.$$

The marginal cdf's of x are:

$$P_x(x \leq 0) = P_x(x = 0) = 0.3.$$

$$P_x(x \leq 1) = P_x(x \leq 0) + P_x(x = 1) = 0.3 + 0.2 = 0.5.$$

$$P_x(x \leq 2) = P_x(x \leq 2) + P_x(x = 2) = 0.5 + 0.5 = 1.$$

The marginal cdf's of y are:

$$P_y(y \leq 0) = P_y(y = 0) = 0.1.$$

$$P_y(y \leq 1) = P_y(y \leq 0) + P_y(y = 1) = 0.1 + 0.5 = 0.6.$$

$$P_y(y \leq 2) = P_y(y \leq 1) + P_y(y = 2) = 0.6 + 0.4 = 1.$$

$$E(x) = \sum_i a_i P_x(x = a_i) = 0P_x(x = 0) + 1P_x(x = 1) + 2P_x(x = 2) =$$

$$(0)(0.3) + (1)(0.2) + (2)(0.5) = 1.2.$$

$$E(y) = \sum_i a_i P_y(y = a_i) = 0P_y(y = 0) + 1P_y(y = 1) + 2P_y(y = 2) =$$

$(0)(0.1) + (1)(0.5) + (2)(0.4) = 1.3.$

Are x and y independent? Do the following statements hold:

$A \subseteq R_x, B \subseteq R_y,$

$P(x \in A, y \in B) = P_x(x = A)P_y(y = B).$

So,

$P(x = 0, y = 0) = 0.1,$

$P_x(x = 0)P_y(y = 0) = (0.3)(0.1) = 0.03,$

Since $0.1 \neq 0.03$, x and y are not independent.

(b) Let $W = 2X^2 + 5$. Compute the pmf and cdf of W. Also, what is $E(W)$?

The range of W is $R_w = \{5, 7, 13\}$.

$$P(w = 5) = \sum_{(i,j):2i^2+5=5} P(x = i, y = j) = P_x(x = 0) = 0.3.$$

$$P(w = 7) = \sum_{(i,j):2i^2+5=7} P(x = i, y = j) = P_x(x = 1) = 0.2.$$

$$P(w = 13) = \sum_{(i,j):2i^2+5=13} P(x = i, y = j) = P_x(x = 2) = 0.5.$$

The cdf of w is:

$P(w \leq 5) = 0.3.$

$P(w \leq 7) = P(w \leq 5) + P(w = 7) = 0.3 + 0.2 = 0.5.$

$P(w \leq 13) = P(w \leq 7) + P(w = 13) = 0.5 + 0.5 = 1.$

$E(w) = 5P(w = 5) + 7P(w = 7) + 13P(w = 13) = (5)(0.3) + (7)(0.2) + (13)(0.5) = 9.4.$

(c) Let $Z = X + Y$. Write down the pmf of Z. Compute $E(Z)$ using this pmf. Verify that $E(Z) = E(X) + E(Y)$. $R_z\{0, 1, 2, 3, 4\}$ The pmf of z is:

$P_z(z = 0) = P(x = 0, y = 0) = 0.1.$

$P(z = 1) = P(x = 0, y = 1) + P(x = 1, y = 0) = 0.2 + 0 = 0.2.$

$P(z = 3) = P(x = 1, y = 2) + P(x = 2, y = 1) = 0.1 + 0.2 = 0.3.$

$P(z = 4) = P(x = 2, y = 2) = 0.3.$

$E(z) = 0P(z = 0) + 1P(z = 1) + 2P(z = 2) + 3P(z = 3) + 4P(z = 4) =$

$(0)(0.1) + (1)(0.2) + (2)(0.1) + (3)(0.3) + (4)(0.3) = 2.5.$

Verification that $E(x) + E(y) = E(z) = 1.2 + 1.3 = 2.5 = 2.5.$

(d) Compute $P(X \leq 1|Y \leq 1)$.

$$P(x \leq 1|y \leq 1) = \frac{P(x \leq 1, y \leq 1)}{P(y \leq 1)} = \frac{P(x = 0, y \leq 1) + P(x = 1, y \leq 1)}{P_y(y \leq 1)} =$$

$$\frac{P(x = 0, y = 0) + P(x = 0, y = 1) + P(x = 1, y = 0) + P(x = 1, y = 1)}{P_y(y \leq 1)} =$$

$$\frac{0.1 + 0.2 + 0 + 0.1}{0.6} = \frac{0.4}{0.6} = \frac{2}{3}.$$

(e) What is the conditional pmf of X given $Y = 1$?

$$P(x = 0|y = 1) = \frac{P(x = 0, y = 1)}{P_y(y = 1)} = \frac{0.2}{0.5} = \frac{2}{5}.$$

$$P(x = 1|y = 1) = \frac{P(x = 1, y = 1)}{P_y(y = 1)} = \frac{0.1}{0.5} = \frac{1}{5}.$$

$$P(x = 2|y = 1) = \frac{P(x = 2, y = 1)}{P_y(y = 1)} = \frac{0.2}{0.5} = \frac{2}{5}.$$

2. Suppose $X_1 \sim Geometric(p)$ and $X_2 \sim Geometric(q)$ and that X_1 and X_2 are independent. Let $Y = \min(X_1, X_2)$. Find the pmf of Y. Start by arguing that $P(Y > k) = P(X_1 > k, X_2 > k)$. Develop this further into an expression for $P(Y > k)$ and use it to obtain the cdf and pmf of Y. What do you notice about $Y's$ pmf? Given an example of a complex experiment and define X_1 and X_2 such that the Geometric distribution is a suitable choice for X_1 and X_2. Identify Y in this experiment. Review the intuition for the form of the Geometric distribution; along the same lines, give an intuitive explanation for the pmf of Y. $P(y > k) = P(x_1 > k, x_2 > k) = P(x_1 > k)P(x_2 > k)$. Find an expression for $P(x_1 > k)$.

$$P(x_1 > k) = P(x_1 = k + 1) + P(x_1 = k + 2) + P(x_1 = k + 3) + \cdots =$$

$$P(x_1 > k) = (1-p)^k p + (1-p)^{k+1} p + (1-p)^{k+2} p + \cdots, \frac{P(x_1 > k)}{(1-p)^k} = p + (1-p)p + (1-p)^2 p + \cdots,$$

$$\frac{P(x_1 > k)}{(1-p)^k p} = 1 + (1-p) + (1-p)^2 + \cdots, \frac{P(x_1 > k)}{(1-p)^k p} = \frac{1}{1-(1-p)} = \frac{1}{p}.$$

$$P(x_1 > k) = (1-p)^k.$$

Find an expression for $P(x_2 > k)$.

$$P(x_2 > k) = P(x_2 = k + 1) + P(x_2 = k + 2) + P(x_2 = k + 3) + \cdots =$$

$$(1-q)^k q + (1-q)^{k+1} q + (1-q)^{k+2} q + \cdots,$$

$$\frac{P(x_2 > k)}{(1-q)^k q} = 1 + (1-q) + (1-q)^2 + \cdots,$$

$$\frac{P(x_2 > k)}{(1-q)^k q} = \frac{1}{1-(1-q)} = \frac{1}{q},$$

$$P(x_2 > k) = (1-q)^k.$$

Substitute back gives:

$$P(y > k) = (1-p)^k (1-q)^k = [(1-p)(1-q)]^k.$$

$$R_y = \{1, 2, 3, ...\}.$$

The pmf of y corresponds to:

$$P(y = 1) = (1-p)(1-q).$$

$$P(y = 2) = [(1-p)(1-q)]^2.$$

And so on. The cdf of y is

$$P(y \le 1) = P(y = 1) = (1-p)(1-q).$$

$$P(y \le 2) = P(y \le 1) + P(y = 2) = (1-p)(1-q) + [(1-p)(1-q)]^2.$$

And so on.

3. Consider the following joint density function for random variables X and Y:

$$f(x,y) = \frac{6}{7}\left(x^2 + \frac{xy}{2}\right), 0 < x < 1, 0 < y < 2.$$

(a) Verify that f is indeed a joint probability density function.

$$\int\int_A f(x,y)\,dx\,dy,$$

where

$$A = \left\{(x,y) : \frac{6}{7}\left(x^2 + \frac{xy}{2}\right) \le f(x,y)\right\} = 1.$$

$$\int\int_A \frac{6}{7}\left(x^2 + \frac{xy}{2}\right)\,dx\,dy = \int_0^2\int_0^1 \frac{6}{7}\left(x^2 + \frac{xy}{2}\right)\,dx\,dy = \int_0^2 \frac{6}{7}\left(\frac{x^3}{3} + \frac{x^2y}{4}\right)\Big|_0^1\,dy =$$

$$\int_0^2 \frac{6}{7}\left(\frac{1}{3} + \frac{y}{4}\right)\,dy = \frac{6}{7}\left(\frac{y}{3} + \frac{y^2}{8}\right)\Big|_0^2 = \left[\frac{6}{7}\left(\frac{2}{3} + \frac{4}{8}\right)\right] = \frac{6}{7}\left(\frac{28}{24}\right) = \frac{4}{4} = 1.$$

(b) Compute the marginal pdf's of X and Y. Verify that the resulting functions are pdf's and use them to compute $E(X)$ and $E(Y)$.

The pdf of x is:

$$f(x) = \int_{-\infty}^{\infty} f(x,y)\,dy = \int_0^2 \frac{6}{7}\left(x^2 + \frac{xy}{2}\right)\,dy = \frac{6}{7}\left(x^2y + \frac{xy^2}{4}\right)\Big|_0^2 = \frac{6}{7}\left(2x^2 + x\right).$$

The pdf of y is:

$$f(y) = \int_{-\infty}^{\infty} f(x,y)\,dx = \int_0^1 \frac{6}{7}\left(x^2 + \frac{xy}{2}\right)\,dx = \frac{6}{7}\left(\frac{x^3}{3} + \frac{x^2y}{4}\right)\Big|_0^1 = \frac{2}{7} + \frac{3y}{14}.$$

Verify the pdf's:

$$\int_{-\infty}^{\infty} f(x)\,dx = 1.$$

$$\int_0^1 \frac{12x^2}{7} + \frac{6x}{7}\,dx = \frac{4x^3}{7} + \frac{3x^2}{7}\Big|_0^1 = \frac{4}{7} + \frac{3}{7} = 1.$$

$$\int_{-\infty}^{\infty} f(y)\,dy = 1. \int_0^2 \frac{2}{7} + \frac{3y}{14}\,dy = \frac{2y}{7} + \frac{3y^2}{28}\Big|_0^2 = \frac{4}{7} + \frac{12}{28} = 1.$$

$$E(x) = \int_{-\infty}^{\infty} xf(x)\,dx = \int_0^1 \frac{12x^3}{7} + \frac{6x^2}{7}\,dx = \frac{12x^4}{28} + \frac{6x^3}{21}\Big|_0^1 = \cdots.$$

$$E(y) = \int_{-\infty}^{\infty} yf(y)\,dy = \int_0^2 y\left(\frac{2}{7} + \frac{3y}{14}\right)\,dy = \frac{y^2}{7} + \frac{y^3}{14}\Big|_0^2 = \frac{4}{7} + \frac{8}{14} = \frac{8}{7}.$$

(c) Are X and Y independent? Does $f(x,y) = f(x)f(y)$? Find one value of x and y that do not satisfy the equation. $x = 1, y = 2$.

(d) Compute $P(Y > \frac{1}{2}|X < \frac{1}{2})$.

$$P\left(y > \frac{1}{2}|x < \frac{1}{2}\right) = \frac{P(x > \frac{1}{2}, x < \frac{1}{2})}{P(x < \frac{1}{2})} = \frac{\int_{\frac{1}{2}}^2\int_0^{\frac{1}{2}} \frac{6}{7}\left(x^2 + \frac{xy}{2}\right)\,dx\,dy}{\int_0^{\frac{1}{2}} \frac{6}{7}\left(2x^2 + x\right)\,dx} =$$

$$\frac{\int_{\frac{1}{2}}^2 \frac{1}{28} + \frac{y}{16}\,dy}{\frac{6}{7}\left(\frac{1}{12} + \frac{1}{8}\right)} = \frac{\left(\frac{2}{28} + \frac{6}{7}\left(\frac{4}{32}\right) - \left(\frac{1}{56} + \frac{1}{128}\right)\right.}{\frac{6}{7}\left(\frac{5}{24}\right)} = \frac{0.154}{0.17857} \approx 0.865.$$

4. Read section 5.8 of your textbook before answering this question. Let X denote the execution time of a randomly selected program. Assume that X is exponentially distributed with parameter Λ where Λ is itself a random variable that is uniformly distributed in the interval (a, b). Compute the cdf of X.[Hint: Write down an expression for $P(X < x|\Lambda = \lambda)$. then use the law of total probability].

$$f(x) = \begin{cases} \lambda e^{-\lambda x}, & \text{if } x > 0. \\ 0, & \text{otherwise.} \end{cases}$$

$$g(\lambda) = \begin{cases} 0, & \text{if } \lambda < a. \\ \frac{1}{b-a}, & \text{if } a < \lambda < b. \\ 0, & \text{if } \lambda \geq b. \end{cases}$$

$$P(X < x|\Lambda = \lambda) = \int_0^x \lambda e^{-\lambda y}\, dy = -e^{-\lambda y}\Big|_0^x = 1 - e^{-\lambda x}.$$

$$P(X < x) = \int_{-\infty}^{\infty} P(X < x|\Lambda = \lambda) g(\lambda) d\lambda = \int_a^b (1 - e^{-\lambda x}) \left(\frac{1}{b-a}\right) d\lambda \cdots$$

4.33 Midterm Exam

1. For any two events $A \subseteq B \subseteq \Omega$, prove that $P(A) \leq P(B)$. Mention which axioms you used in your proof.

2. A card is drawn from a pack and inserted into a second pack. Then, a card is drawn from the *second* pack. Define the following events: let A be the event that the second card is a Spade; let B_1 be the event that the first card is a Spade. Compute $P(A)$ and $P(B_1|A)$. [Hint: you will need the law of total probability and Baye's rule]. A = 2-nd card is a spade. B_1 = 1-st card is a spade. $\Omega_1 = \{1, 2, 3, ..., 52\}$. $\Omega_2 = \{1, 2, 3, ..., 52\}$. $\Omega = \Omega_1 \times \Omega_2 = \{(x, y) : x \in \Omega_1; y \in \Omega_2\}$. $A = \{(0, 1), (0, 2), (0, 3), ..., (0, 13)\}$. $P(B_1) = \frac{13}{52}$. By the law of total probability,

$$P(A|B_1)P(B_1) + P(A|B_1^c)P(B_1^c) = \frac{14}{53}\left(\frac{13}{52}\right) + \frac{13}{53}\left(\frac{39}{52}\right).$$

First compute $P(A) = \sum_{i=1}^{n} P(A|B_i)P(B_i)$. Then, compute $P(B_1|A) = \frac{P(A|B_1)P(B_1)}{P(A)}$. The probability of A has already been computed. Then,

$$P(B_1|A) = \frac{P(A|B_1)P(B_1)}{P(A)} = \frac{\left(\frac{14}{53}\right)\left(\frac{13}{52}\right)\left(\frac{13}{52}\right)}{\left(\frac{14}{53}\right)\left(\frac{13}{52}\right) + \left(\frac{13}{53}\right)\left(\frac{39}{52}\right)}.$$

3. X_1 and X_2 are independent Bernoulli random variables, both with parameter p. Name the distribution of $Z = X_1 + X_2$. What is the range of Z?

   $x_1 \in \{0, 1\}$. $P(x_1 = 1) = p$, $P(x_1 = 0) = (1 - p)$. $x_2 \in \{0, 1\}$. $P(x_2 = 1) = p$, $P(x_2 = 0)](1 - p)$. $R_z = \{0, 1, 2\}$.

$$P(Z = 0) = P(x_1 = 0) + P(x_2 = 0) = (1 - p) + (1 - p) = 2(1 - p).$$

$$P(Z = 1) = [p + (1 - p) + (1 - p) + p] = 2.$$

$$P(Z = 2) = P(x_1 = 1) + P(x_2 = 1) = p + p = 2p.$$

   $Z \sim Binomial(2, p)$.

4. The continuous random variable X has a density function given by

$$f(x) = \begin{cases} cx, & 0 < x < 10. \\ 0, & \text{otherwise.} \end{cases}$$

(a) What value of c will make this a valid probability density function?

$$\int_{-\infty}^{\infty} f(x)\,dx = 1,$$

$$\int_{0}^{10} cx\,dx = 1,$$

$$\left.\frac{cx^2}{2}\right|_0^{10} = 1,$$

$$\frac{c100}{2} - 0 = 1,$$

$$c = \frac{2}{100} = \frac{1}{50}.$$

At $c = \frac{1}{50}$, $f(x)$ is a probability density function.

(b) Compute $E(X)$.

$$E(x) = \int_{-\infty}^{\infty} xf(x)\,dx,$$

$$\int_0^{10} x\left(\frac{1}{50}\right)x\,dx = \frac{1}{50}\int_0^{10} x^2\,dx = \left.\frac{x^3}{(50)(3)}\right|_0^{10} = \frac{1000}{150} - 0 = \frac{100}{15}.$$

5. The joint density of X and Y is given by

$$f(x,y) = \begin{cases} e^{-(x+y)}, & x > 0, y > 0. \\ 0, & \text{otherwise.} \end{cases}$$

Answer the following questions, leaving your answers in the form of definite integrals(with the proper limits of the integrals written in). *Do not evaluate the integrals.*

(a) What is the marginal pdf of Y?

$$f(y) = \int_{-\infty}^{\infty} f(x,y)\,dx = \int_0^{\infty} e^{-(x+y)}\,dx = -e^{-(x+y)}\Big|_0^{\infty}, x > 0, y > 0.$$

$e^{-y}, x > 0, y > 0.$

(b) What is $P(X < 5|Y > 10)$?

$$P(x < 5|y > 10) = \frac{\int_B \int_A f(x,y)\,dx\,dy}{P(y > 10)} = \frac{\int_{10}^{\infty}\int_0^5 e^{-(x+y)}\,dx\,dy}{\int_1^{\infty} e^{-y}\,dy}.$$

6. The joint pmf of X and Y is tabulated below:

x/y	1	2
1	0.2	0.1
2	0.1	0.6

(a) Compute the marginal pmf of X.

$$P_x(x = 1) = P(x = 1, y = 1) + P(x = 1, y = 2) = 0.2 + 0.1 = 0.3.$$

$$P_x(x = 2) = P(x = 2, y = 1) + P(x = 2, y = 2) = 0.1 + 0.6 = 0.7.$$

(b) Compute $E(X)$.

$$E(x) = \sum_{j \in R_y} a_i P(x = a_i, y = b_j).$$

$$E(x) = (1)P(_x(x = 1) + (2)P_x(x = 2) = (1)(0.3) + (2)(0.7) = 1.7.$$

(c) Determine whether X and Y are independent.

$$P_x(x = a_i)P_y(y = b_j) = P(x = a_i, y = b_j).$$

$$P_y(y = 1) = P(y = 1, x = 1) + P(y = 1, x = 2) = 0.2 + 0.1 = 0.3.$$

$$P_y(y = 2) = P(y = 2, x = 1) + P(y = 2, x = 2) = 0.1 + 0.6 = 0.7.$$

x and y are not independent at $P_x(x = 1)P_y(y = 1) \neq 0.2 \neq P(x = 1, y = 1)$.

4.34 Theory of Probability

4.34.1 The Normal Distribution and the Central Limit Theorem

w_1, w_2.

$$P\left(\frac{s_n(w_1)}{n} \to \mu\right) = 1,\ \ P\left(\frac{s_n(w_2)}{n} \to \mu\right) = 1,$$

for $n = 1000$. How far are we from the mean,

$$P\left(\left|\frac{s_n}{n} - \mu\right| \leq \epsilon\right) =?$$

The Normal distribution is $Z \sim N(\mu, \sigma^2)$, if the pdf of z is

$$f_z(x) = \frac{e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}}{\sqrt{2\pi}\sigma}, -\infty < x < \infty.$$

$E(z) = \mu$, $Var(z) = \sigma^2$. When $Z \sim N(0, 1)$, then

$$f_z(x) = \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}},$$

and,

$$F_z(y) = P(Z \leq Y) = \int_{-\infty}^{\infty} f_z(x)\,dx.$$

The notation used is $\Phi(y) = F_z(y)$ for $Z \sim N(0, 1)$. That is called the *standard normal distribution.* Properties of z.

1. $x_1, x_2, ..., x_n$ with $x_i \sim N(\mu, \sigma^2)$. Then,

$$s_n = \sum_{i=1}^{n} x_i \sim N\left(\sum_{i=1}^{n} \mu_i, \sum_{i=1}^{n} \sigma_i^2\right),$$

where the $x_i' s$ are independent.

2. $x \sim N(\mu, \sigma^2)$. Then,

$$Z = \frac{x - \mu}{\sigma} \sim N(0, 1).$$

This is called the *scaling property.*

Example: Suppose $x \sim N(\mu, \sigma^2)$. We want $P(x < a)$.

$$P(x < a) = P\left(\frac{x-\mu}{\sigma} < \frac{a-\mu}{\sigma}\right) = P\left(Z < \frac{a-\mu}{\sigma}\right) = \Phi\left(\frac{a-\mu}{\sigma}\right).$$

Example: Find $P(a < x < b)$, given $x \sim N(\mu, \sigma^2)$.

$$P(a < x < b) = P(x < b) - P(x < a) = \Phi\left(\frac{b-\mu}{\sigma}\right) - \Phi\left(\frac{a-\mu}{\sigma}\right).$$

4.34.2 Central Limit Theorem

$x_1, x_2, ...$ is an iid sequence meaning $\mu < \infty$ and $\sigma^2 < \infty$. Let $S_n = \sum_{i=1}^{n} x_i$ and $Z \sim N(0, 1)$. Then,

1. $\frac{s_n - n\mu}{\sqrt{n}\sigma} \to Z$, in distribution.
2. $\frac{\frac{s_n}{n} - \mu}{\frac{\sigma}{\sqrt{n}}} \to Z$ in distribution. $\frac{s_n}{n} \to \mu$ and $\left(\frac{s_n}{n} - \mu\right) \to 0$.

Example: In measurements of program calculation times, $\mu = 4$ seconds and $\sigma^2 = 100$. x_i is the execution time of the i-th program. $s_n = \sum_{i=1}^{n} x_i$. What is $P(s_n > 100)$? Use the Central Limit Theorem.

$$W_n = \frac{s_n - n\mu}{\sqrt{n}\sigma} \to Z.$$

Then,

$$P(s_n > 100) = P\left(\frac{s_n - n\mu}{\sqrt{n}\sigma} > \frac{100 - n\mu}{\sqrt{n}\sigma}\right) = P\left(Z > \frac{100 - n\mu}{\sqrt{n}\sigma}\right) = 1 - \Phi\left(\frac{100 - n\mu}{\sqrt{n}\sigma}\right).$$

At $n = 16$, we have,

$$1 - \Phi\left(\frac{100 - 16(4)}{4(10)}\right).$$

4.34.3 Point Estimation and Confidence Intervals

Measurements $x_1, x_2, ...$

$$\hat{\mu} = \frac{x_1 + x_2 + \cdots + x_n}{n} = \frac{s_n}{n}, \quad \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{\mu})^2.$$

Two important questions:

1. What is the true value of μ for which

$$P\left(\left|\frac{s_n}{n} - \mu\right| < \delta\right) > 0.95?$$

2. Given n, what is the smallest δ for which

$$P\left(\left|\frac{s_n}{n} - \mu\right| < \delta\right) > 0.95?$$

Example: $x_1, x_2, ...$ is a Bernoulli sequence (i.e. $x \in \{0, 1\}$). Suppose $n = 100$. Say, $\hat{\mu} = 0.49$, and $\hat{\sigma}^2 = 0.01$. What is the 95% confidence interval? The first assumption is that we have an iid sequence.

$$P\left(\left|\frac{s_{100}}{100} - \mu\right| < \delta\right) > 0.95 \approx N(0,1), \quad \frac{\frac{s_{100}}{100} - \hat{\mu}}{\hat{\sigma}\sqrt{100}} \approx \frac{\frac{s_{100}}{100} - \mu}{\sigma\sqrt{100}} \sim N(0,1).$$

$$P\left(\mu - \delta < \frac{s_{100}}{100} < \mu + \delta\right) > 0.95 \Rightarrow P\left(\frac{\mu - \delta - \mu}{\frac{\sigma}{10}} < \frac{\frac{s_{100}}{100} - \mu}{\frac{\sigma}{10}} < \frac{\mu + \delta - \mu}{\frac{\sigma}{10}}\right) > 0.95 \Rightarrow$$

$$P\left(\frac{-\delta}{\frac{\sigma}{10}} < \frac{\frac{s_{100}}{100} - \mu}{\frac{\sigma}{10}} < \frac{\delta}{\frac{\sigma}{10}}\right) > 0.95 \Rightarrow P\left(\frac{-\delta}{\frac{\hat{\sigma}}{10}} < \frac{\frac{s_{100}}{100} - \hat{\mu}}{\frac{\hat{\sigma}}{10}} < \frac{\delta}{\frac{\hat{\sigma}}{10}}\right) > 0.95 \Rightarrow$$

$$P\left(\frac{-\delta}{\frac{\hat{\sigma}}{10}} < z < \frac{\delta}{\frac{\hat{\sigma}}{10}}\right) > 0.95 \Rightarrow P\left(\frac{-\delta}{0.01} < z < \frac{\delta}{0.01}\right) > 0.95 \Rightarrow$$

$$\Phi\left(\frac{\delta}{0.01}\right) - \Phi\left(\frac{-\delta}{0.01}\right) > 0.95 \Rightarrow 2\Phi\left(\frac{\delta}{0.01}\right) - 1 > 0.95.$$

4.34.4 Law of Large Numbers

Example: A coin flip. Let

$$x_i = \begin{cases} 1, & \text{if } i\text{-th flip is heads.} \\ 0, & \text{otherwise.} \end{cases}$$

$E(x_i) = 0P(x = 0) + 1P(x = 1) = \frac{1}{2}$. $x_i \sim Bernoulli(\frac{1}{2})$. Define $s_n = \sum_{i=1}^{n} x_i =$ number of heads. Observe $\frac{\text{\# of 1's}}{\text{\# of trials}} \to \frac{1}{2}$. $s_n \approx \frac{s_n}{n} \to \frac{1}{2}$.

Example: Suppose $x_i \sim U(a, b)$ What does $\frac{s_n}{n}$ approach? $E(x_i) = \frac{a+b}{2}$.

4.34.5 Sample Paths and Modes of Convergence

Recall the 3 coin flips example.

1. a random variable is a function, $x : \Omega \to \Re$.

2.

$w \in \Omega$	$P(w)$	$x_1(w)$	$x_2(w)$	$x_3(w)$	$s_3(w)$
(H,H,H)	$\frac{1}{8}$	1	1	1	3
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	.
(T,T,T)	$\frac{1}{8}$	0	0	0	0

$$P(x_2 = 1) = P(\{w \in \Omega : x_2(w) = 1\}) = \frac{4}{8} = \frac{1}{2}.$$

$$P(x_2 = 0) = \frac{4}{8}.$$

The joint pmf is $P(x_1 = 1, x_2 = 1, x_3 = 1) = \frac{1}{8}$. $\Omega = \Omega_1 \times \Omega_2 \times \Omega_3$. $\Omega_1 = \{H, T\}$. Given n $x(w)'s$, $\Omega = \Omega_1 \times \Omega_2 \times \cdots \times \Omega_n$. Fix $w \in \Omega$ and observe $x_1(w), x_2(w), x_3(w), ...$ that is a real number sequence. W is known as a *sample path, sample run, or sample track.*

$s_n(w) = \sum_{i=1}^n x_i(w) = s_1(w), s_2(w), s_3(w), ...$ $\frac{s_n(w)}{n} = \frac{1}{n}\sum_{i=1}^n x_i(w) = \frac{s_1(w)}{1}, \frac{s_2(w)}{2}, ...$ Does $x_n(w)$ converge to anything? Does $s_n(w)$ converge to anything? Does $\frac{s_n(w)}{n}$ converge to anything? eg. $W = (H, H, H, ..., H)$. $x_n(w) \to 1$. $s_n(w) \to \infty$. $\frac{s_n(w)}{n} \to \frac{n}{n} = 1$.

Example: $W = (H, T, H, T, H, ...)$.

$$x_n(w) = \begin{cases} 0, & \text{if } n \text{ is even.} \\ 1, & \text{if } n \text{ is odd.} \end{cases}$$

x_n does not converge.

$$s_n(w) = \begin{cases} \frac{n}{2}, & \text{if } n \text{ is even.} \\ \frac{n-1}{2}, & \text{if } n \text{ is odd.} \end{cases}$$

$$\frac{s_n(w)}{n} \to \frac{1}{2} = \begin{cases} \frac{1}{2}, & \text{if } n \text{ is even.} \\ \frac{1-\frac{1}{n}}{2}, & \text{if } n \text{ is odd.} \end{cases}$$

Let $A = \{\text{all } w's : \frac{s_n}{n} \to \frac{1}{2}.\}$ Let $B = \{\text{all other } w's.\} = \Omega - A$. Then, $P(A) = 1$.

4.34.6 Strong Law of Large Numbers

Let $x_1, x_2, x_3, ...$ be a sequence of random variables such that:

1. $x_1, x_2, x_3, ...$ are independent.
2. $x_1, x_2, x_3, ...$ are identically distributed.
3. $E(x_i) < \infty$ and $E(x_i^2) < \infty$.

Let $\mu = E(x_i)$, and $s_n = \sum_{i=1}^n x_i$. Then,

$$P\left(w : \frac{s_n(w)}{n} \to \mu\right) = 1.$$

To say the strong law converges in the weak sense is to say,

$$\forall \epsilon > 0, P\left(\left|\frac{s_n}{n} - \mu\right| > \epsilon\right) \to 0.$$

Example: Let $x_1, x_2, ...$ be an iid sequence. $s_i \sim U(a, b)$. $s_n = \sum_{i=1}^n x_i$. What does $\frac{s_n}{n}$ approach? $\mu = E(x_1)$. $\frac{s_n}{n} \to \mu = \frac{a+b}{2}$. Therefore,

$$P\left(w : \frac{s_n}{n} \to \mu = \frac{a+b}{2}\right) = 1.$$

Find a sequence such that $\frac{s_n}{n}$ does not approach μ. $w' = (a, a, a, ...)$.

Example: $x_1, x_2, ...$ is iid, $x_i \sim Exp(\lambda)$. $\frac{s_n}{n} \to \frac{1}{\lambda}$. Therefore,

$$P\left(w : \frac{s_n}{n} \to \frac{1}{\lambda}\right) = 1,$$

except for $w' = (20^{100}, 20^{100}, 20^{100}, ...)$.

4.34.7 Types of Convergence

$s_1, \frac{s_2}{2}, \frac{s_3}{3}, ...$ is not an iid sequence. Rename the sequence $z_n = \frac{s_n}{n}$; then, $z_1, z_2, z_3, ...$ is a sequence of random variables. Types of convergence:

1. Strong Convergence - $Z_n \to L$ almost surely if $P(w : Z_n(w) \to L) = 1$

   Example: $x_1, x_2, ...$ is an iid sequence. $\mu = E(x_i)$. Let $z_n = \frac{s_n}{n}$. Then by the strong law of large numbers, $z_n \to \mu$ almost surely.

2. Weak Convergence - $Z_n \to L$ in probability if $\forall \epsilon > 0$, $P(|z_n - L| > \epsilon) \to 0$. $z_1, z_2, z_3, ...$ is any sequence(not just an iid sequence). Let,

$$a_1 = P(|z_1 - L| > \epsilon)$$

$$a_2 = P(|z_2 - L| > \epsilon)$$

$$...$$

$$a_n = P(|z_n - L| > \epsilon)$$

$$...$$

   $a_1, a_2, a_3, ...$ is a real numbered sequence.

   Example: Suppose $z_n \sim Bernoulli(\frac{1}{n})$. The claim is $z_n \to 0$ in probability.

$$z_1 \sim Bernoulli(1),\ z_2 \sim Bernoulli\left(\frac{1}{2}\right),\ z_3 \sim Bernoulli\left(\frac{1}{3}\right) ...$$

   Show $P(|z_n - L| > \epsilon) \to 0, \forall \epsilon > 0$.

$$P(|z_n - 0| > \epsilon) = P(z_n > 0) = P(z_n = 1) = \frac{1}{n}.$$

   Thus, $P(z_n = 1) \to 0$.

   Example: $z_n \sim U(0, \frac{b}{n})$. The claim is that $z_n \to 0$ in probability.

$$z_1 \sim U(0, b),\ z_2 \sim U\left(0, \frac{b}{2}\right),\ z_3 \sim U\left(0, \frac{b}{3}\right), ...$$

   Show $P(|z_n - 0| > \epsilon) \to 0, \forall \epsilon > 0$.

$$P(z_n \in (\epsilon, \frac{b}{n})) = \int_{\epsilon}^{\frac{b}{n}} \frac{1}{\frac{b}{n} - 0}\, dx,$$

for $\frac{b}{n} > \epsilon$. 0, otherwise. Evaluating the integral yields:

$$\frac{\frac{b}{n} - \epsilon}{\frac{b}{n}}, \frac{b}{n} > \epsilon.$$

0 otherwise. Moreover, $a_n = P(|z_n - 0| > \epsilon)$.

The main result is that if $z_n \to L$ almost surely, then $z_n \to L$ in probability.

3. Convergence in Distribution - Consider a sequence $z_1, z_2, ...$ of random variables. Let $F_n(y)$ be the cdf of z_n, and $F(y)$ be the cdf of z. Suppose $F_n(y) \to F(y)$. Then, $z_n \to z$ in distribution. This is the convergence of functions to a function.

4.34.8 Variance

$$Var(x) = \int_{-\infty}^{\infty} (x - \mu)^2 f(x)\, dx,$$

where $\mu = E(x)$. Properties of variances:

1. $Var(x) = E(x^2) - [E(x)]^2$.
2. $Var(ax + b) = a^2 Var(x)$.
3. if $x_1, x_2, ..., x_n$ are independent, then $Var(x_1 + x_2 + \cdots + x_n) = Var(x_1) + Var(x_2) + \cdots + V(x_n)$.

Example: $x \sim U(a, b)$. $E(x) = \frac{a+b}{2}$.

$$E(x^2) = \int_a^b \frac{x^2}{b-a}\, dx = \frac{1}{3}\left(\frac{b^3 - a^3}{b - a}\right) = \frac{1}{3}(b^2 + ab + a^2).$$

$$Var(x) = E(x^2) - [E(x)]^2 = \frac{1}{3}(a^2 + ab + b^2) - \left(\frac{a+b}{2}\right)^2 = \frac{(b-a)^2}{12}.$$

4.34.9 Chebyshev's Inequality

Suppose $E(x) = \mu < \infty$, and $Var(x) = \sigma^2 < \infty$. Then, for $\epsilon > 0$, $P(|x - \mu| \geq \epsilon) \leq \frac{\sigma^2}{\epsilon^2}$.

Proof:(continuous case)

$$P(|x - \mu| \geq \epsilon) = \int_{|(x-\mu)| \geq \epsilon} f(x)\, dx = \int_{|x-\mu|^2 \geq \epsilon^2} f(x)\, dx = \int_{|x-\mu|^2 \geq \epsilon^2} \frac{\epsilon^2}{\epsilon^2} f(x)\, dx \leq$$

$$\int_{|x-\mu|^2 \geq \epsilon^2} \frac{(x-\mu)^2}{\epsilon^2} f(x)\, dx \leq \frac{1}{\epsilon^2} \int_{-\infty}^{\infty} (x - \mu)^2 f(x)\, dx = \frac{\sigma^2}{\epsilon^2}.$$

4.34.10 Weak Law of Large Numbers

Let $x_1, x_2, ...$ be an iid sequence.

$$s_n = \sum_{i=1}^{n} x_i, \forall \epsilon \geq 0, P\left(\left|\frac{s_n}{n} - \mu\right| \geq \epsilon\right) \to 0.$$

Proof:

Let $z_n = \frac{s_n}{n}$. Then,

$$P(|z_n - E(z_n)| \geq \epsilon) \leq \frac{Var(z_n)}{\epsilon^2}.$$

$$E(z_n) = E\left(\frac{s_n}{n}\right) = \frac{1}{n}E(s_n) = \frac{1}{n}E(x_1 + x_2 + \cdots + x_n) = \mu$$

$$Var(z_n) = \frac{Var(x_1 + x_2 + \cdots + x_n)}{n} = \frac{1}{n^2}Var(x_1 + x_2 + \cdots + x_n) =$$

$$\frac{1}{n^2}(Var(x_1) + Var(x_2) + \cdots + Var(x_n)) = \frac{1}{n^2}(n\sigma^2) = \frac{\sigma^2}{n}.$$

Thus,

$$P\left(\left|\frac{s_n}{n} - \mu\right| \geq \epsilon\right) \leq \frac{\sigma^2}{n\epsilon^2}.$$

$$\frac{\sigma^2}{n\epsilon^2} \to 0.$$

Therefore,

$$P\left(\left|\frac{s_n}{n} - \mu\right| \geq \epsilon\right) \to 0.$$

In 1713, the Weak Law of Large Numbers for Bernoulli random variables was proven by Jacob Bernoulli. In the 1930's, the general Weak Law of Large Numbers was proven by Chebyshev and Khintchine. The Strong Law of Large Numbers for Bernoulli random variables was proven by E. Bore, and the general Strong Law of Large Numbers was proven by Kolmogorov.

Example: The use of the Strong Law of Large Numbers. Throw a die.

$$\frac{\#6's}{\#\text{ tries}} \to \frac{1}{6}.$$

$$x_i = \begin{cases} 1, & \text{if } i\text{-th throw is a 6.} \\ 0, & \text{otherwise.} \end{cases}$$

$E(x_i) = 0E(x_i = 0) + 1E(x_i = 1) = \frac{s_n}{n} \to E(x_i)$.

Example:

$$P\left(w : \frac{s_n(w)}{n} \to \mu\right) = 1.$$

$$w_1 = \frac{s_n(w_1)}{n} \to \mu.$$

$$w_2 = \frac{s_n(w_2)}{n} \to \mu.$$

$$\mu = 0.5.$$

For the sequence (0.1, 0.9, 0.2, 0.8,...), $\frac{s_{100}(w_1)}{100} = 0.51$. For the sequence (0.99, 0.98, 0.999,...), $\frac{s_{100}(w_2)}{100} = 0.99$. $\frac{s_{1000}}{1000} \approx \mu$.

4.34.11 Example of the Central Limit Theorem

Example: Most of estimates on disk access times, $\hat{\mu} = 10$, $\hat{\sigma} = 16$. We would like to be sure of being within 5% of the mean. How many samples are needed? Let $x_1, x_2, \ldots$ be the measurements.

$$\frac{s_n}{n} = \frac{1}{n}\sum_{i=1}^{n} x_i.$$

Let μ be the true mean and σ^2 be the true variance. We want

$$\mu - 0.05\mu < \frac{s_n}{n} < \mu + 0.05\mu.$$

$$P\left(\mu - 0.05\mu < \frac{s_n}{n} < \mu + 0.05\mu\right) > 0.95.$$

The central limit theorem says that,

$$W_n = \frac{\frac{s_n}{n-\mu}}{\frac{\sigma}{\sqrt{n}}} \to Z$$

in distribution, where $Z \sim N(0,1)$. $W_n \approx N(0,1)$.

$$\frac{\frac{s_n}{n} - \hat{\mu}}{\frac{\hat{\sigma}}{\sqrt{n}}} \approx N(0,1).$$

$$P\left(\frac{-0.05\hat{\mu}}{\frac{\hat{\sigma}}{\sqrt{n}}} < \frac{\frac{s_n}{n} - \hat{\mu}}{\frac{\hat{\sigma}}{\sqrt{n}}} < \frac{0.05\hat{\mu}}{\frac{\hat{\sigma}}{\sqrt{n}}}\right) > 0.95.$$

This is approximately the value of n when n is chosen so that

$$P\left(\frac{-0.05\hat{\mu}}{\frac{\hat{\sigma}}{\sqrt{n}}} < Z < \frac{0.05\hat{\mu}}{\frac{\hat{\sigma}}{\sqrt{n}}}\right) > 0.95 \Rightarrow P\left(\frac{-0.05(10)}{\frac{4}{\sqrt{n}}} < Z < \frac{0.05(10)}{\frac{4}{\sqrt{n}}}\right) > 0.95.$$

$$2\Phi\left(\frac{0.5\sqrt{n}}{4}\right) - 1 > 0.95 \Rightarrow \frac{0.5(\sqrt{n})}{4} > 1.96 \Rightarrow n > 245.8.$$

At least 246 measurements should be taken.

4.35 Programming Assignment

In this programming assignment you will implement a linked list and field accesses to the list in an efficient manner. There are no additions or deletions made to the list, which itself will be provided to you initially. Instead you will only have to access elements and change certain values. The list itself may be *rearranged* to provide faster access time. The following contains a description of the assignment and what you are expected to submit.

We are going to keep track of the *share prices* of ten corporations as they change daily at the New York Stock Exchange. The corporations are named 'A' to 'J.' The **record** structure **corporation** is used to store the name(**name**) and share price(**share_price**) of each corporation. Initially, you will be provided with a linked list with the ten corporations in alphabetical order (this can be seen, and you are encouraged to do this, by examining the code in procedure **initialize**). Your program will read in **num_accesses** and generate this many random accesses to the linked list. For example, if **num_accesses=** 10, then 10 accesses should be generated. Each access is to be generated by calling the function **next_record,** which returns a record of type **corporation.** The record will contain a name and the latest(randomly generated) share price. The linked list is then to be searched for the element corresponding to the named corporation and the share price. The linked list is then to be searched for the element corresponding to the named corporation and the share price updated. You will perform **num_accesses** updates to the list(10 updates, in the above example).

We are interested in recording access time - in particular, average access times. For the n-th access, let Y_n denote the *position* of the corresponding element within the list. For example, if the second access is to corporation 'D' and 'D' happens to be in the 6th position in the linked list, then $Y_2 = 6$. We will use $\hat{\mu} = \frac{S_k}{k} = \frac{1}{k}\sum_{n=1}^{k} Y_n$ to approximate the mean access time(here, $k =$**num_accesses** in the program). You are to also estimate the variance using only the first **max_variance_samples** or k samples, whichever is smaller. Let's use m to denote min(k,**max_variance_samples**). Next, compute an estimate of the variance using

$$\hat{\sigma}^2 = \frac{1}{m-1}\sum_{n=1}^{m}(Y_n - \hat{\mu})^2.$$

With each access made, you are permitted to rearrange the list. Implement the following strategies:

- *Null strategy.* Do nothing to the list - leave it the same as when you started.
- *Head of Line.* Move the currently accessed element to the front of the list.
- *Swap.* Move the currently accessed element by one place towards the front of the list, i.e., swap it with the next element in front. Of course, with both *Head of Line* and *Swap,* if the currently accessed element is the very first one, then one doesn't need to move it.
- *Any other strategy of your choice.* Try to beat the above strategies with one of your own.

For each strategy you should print out the mean access time for the given sample size(**num_accesses**).

Deliverables for this assignment:
You should hand in *TWO neat* copies(one for my records) of:

- Supporting documentation for the program: a paragraph describing your code.
- A *complete* listing of your code together with procedures I have supplied. Your code will contain copious in-line documentation, of course.
- Explain your strategy and the rationale for it. Compare the list manipulation overhead of your strategy with the overhead for the other strategies.
- *Annotated* output from your program: Repeat the following for
  num_accesses = 10, 100, 1000 and 50,000.

  1. For each strategy print the initial list(before the first access).
  2. For each strategy print out the estimated mean access time and variance and also, print out the list after the last access.
  3. Estimate the access probability for corporation 'A', i.e. the probability that a randomly generated access is for corporation 'A.'

  Use the same starting seed for each run, i.e., execute put_seed(7774755) before each run for each strategy.

- Answer the following questions, assuming that successive calls to **x_random** generate independent random values from a $U(0, 1)$ distribution.

  1. Identify one iid sequence and one non-iid sequence in the assignment. Name these sequences using capital letters(as we have been doing in class).
  2. Show how the Strong Law of Large Numbers may be used for the iid sequence above.

3. Consider the *Null strategy.* Suppose we want to be 95% sure that the estimated mean lies within 5% of the true mean access time - how many samples(accesses) will be needed? Show how the Central Limit Theorem is used to provide an estimate of this number. Explicitly point out any approximations that you need to make.
4. Could a similar analysis(of the number of samples required) be made for the other strategies? Are further approximations/ assumptions needed? Explain.
5. Pick out a sequence of random variables in the assignment which converges *almost surely* to a limit. What is the limit? Give an example of a sample path on which the sequence converges and one on which the sequence does not converge.
6. Let X be the random variable denoting the number of calls to **next_record** required to make the first access to corporation 'A'(i.e. the first time an update is needed for 'A'). What is the name of the distribution of X? Compute $E(s_x)$ in closed form.

```
program second_assignment(input, output);
(* the following program gathers some statistics and probabilities of
techniques used to search a list *)

const
     m = 2147483647; (* constant used in random # generator *)
     num_corp = 10;  (* # of corporations *)
     max_variance_samples = 100; (* limit the number of samples for
                                    variance estimation *)

type
     ptr_to_corporation = ^corporation;
     corporation = record
          name: 'A'..'Z'; (* name of each corporation *)
          share_price: real; (* it's share price *)
          next: ptr_to_corporation; (* pointers *)
     end;

     arraytype = array[1..num_corp] of ptr_to_corporation;

var
     p,s: array[0..num_corp] of real; (* true access probabilities
                                         and cdf *)
     x_seed: integer; (* seed of random number generator *)
     ord_A: integer;  (* a convenience for using chr function *)
     sample: array[1..max_variance_samples] of real; (* array of results
                          for variance calculation *)
     front: ptr_to_corporation; (* first element of the list *)
     num_accesses: integer; (* counter *)

(* random number generator *)
function x_random: real;
const
     a = 16807;
     q = 127773;
     r = 2836;
var
     t, lo, hi: integer;
begin
```

```
     hi:= x_seed div q;
     lo:= x_seed - q*hi;
     t:= a*lo - r*hi;
     if t>0 then x_seed:= t
     else x_seed:= t+m;
     x_random:= x_seed/m;
end;

procedure put_seed(x: integer);
begin
     if (0<x) and (x<m) then x_seed:= x;
end;

(* initialize random number generator and data structure *)
procedure initialize;
var
     i: integer;
     sum, c: real;
     prev, current: ptr_to_corporation;
begin
     sum:= 0;
     put_seed(7774755); (* initialize random number generator *)
     ord_A:= ord('A') - 1;
     write('enter number of accesses: ');
     readln(num_accesses);
     (* i's setting the values of access probabilities. first the pmf *)
     p[num_corp]:= 0.15;
     p[num_corp-1]:= 0.121;
     p[num_corp-2]:= 0.12;
     for i:= num_corp-3 downto 1 do sum:= sum+1.0/i;
     c:= 0.609/sum;
     for i:= num_corp-3 downto 1 do p[i]:= c/i;
     (* now the cdf *)
     s[0]:= 0;
     for i:= 1 to num_corp do s[i]:= s[i-1] + p[i];
     (* create initial list in the order A, B, ..., J with 0.0 share price *)
     new(prev);
     front:= prev;
     prev^.name:= 'A';
     prev^.share_price:= 0.0;
     i:= 2;
     while i<=num_corp do
     begin
          new(current);
          current^.name:= chr(ord_A+i);
          current^.share_price:= 0.0;
          prev^.next:= current;
          i:= i+1;
     end;
     new(current^.next);
     current^.next^.next:= nil;
end; (* of initialize *)

(* randomly generates a record with new share price *)
```

```
function next_record: corporation;
var
     u: real;
     j: integer;
     corp: corporation;
begin
     u:= x_random;
     j:= 1;
     while (u>s[j]) and (j<num_corp) do j:= j+1;
     corp.name:= chr(ord_A+j);
     corp.share_price:= 10*x_random;
     next_record:= corp;
end; (* of next_record *)

procedure main_body;
var
     a_count: integer; (* # times 'A' accessed *)
     count: integer;   (* # accesses *)
     k: integer;       (* # references to next_record *)
     y: integer;       (* sum of # accesses *)
     corp_oration: corporation; (* record to be updated *)
     dummy: ptr_to_corporation;
     m: integer;       (* # of samples *)
     var_count: array[1..max_variance_samples] of integer;
                       (* variance sample *)
     mean, variance: real (* of # accesses *)
     i: integer;       (* a counter *)

  procedure print_list(l: ptr_to_corporation);
  (* the following procedure prints a linked list *)
  var
     temp: ptr_to_corporation;
  begin
     while temp^.next<>nil do
     begin
          writeln('Corporation ',temp^.name,' share price is ',
              temp^.share_price:6:2);
          temp:= temp^.next;
     end;
  end; (* of print_list *)

  function linear_search(name: corporation;
        var node:ptr_to_corporation):integer;
  (* the following function performs a linear search for the name
  of a corporation in the list pointed to by 'front' *)
  var
     temp: ptr_to_corporation;
     i: integer;
  begin
     i:= 1;
     if name.name='A' then a_count:= a_count+1;
     temp:= front;
     while (temp^.name<>name.name) and (temp^.next<>nil) do
```

```
   begin
        i:= i+1;
        temp:= temp^.next;
   end;
   temp^.share_price:= name.share_price;
   linear_search:= i;
   node:= temp;
end;

procedure swap(var node1, node2: ptr_to_corporation);
(* the following procedure interchanges two nodes in a singular
linked list *)
var
   temp1, temp2: ptr_to_corporation;
begin (* of swap *)
   if (node1<>nil) and (node2<>nil) then
   if node1^.name<>node2^.name then
   begin
        temp:= node1;
        temp^.name:= node1^.name;
        temp^.share_price:= node1^.share_price;
        temp^.next:= node1^.next;
        node1^.name:= node2^.name;
        node1^.share_price:= node2^.share_price;
        node1^.next:= node2^.next;
        node2^.name:= temp^.name;
        node2^.share_price:= temp^.share_price;
        node2^.next:= temp^.next;
   end;
end;(* of swap *)


function search_and_move(name: corporation):integer;
(* the following function performs a linear search for an element
in a linked list and moves the element that was searched for
one position to the front of the list *)
var
   temp, temp2: ptr_to_corporation;
begin
   temp:= nil;
   search_and_swap:= linear_search(name, temp);
   temp2:= front;
   while (temp2^.next<>temp) and (temp2^.next<>nil) do
        temp2:= temp2^.next;
   if temp2^.next=nil then temp2:= nil;
   if temp^.next=nil then temp:= nil;
   swap(temp, temp2);
end;


function min(m,n: integer):integer;
(* the following function returns the minimum value of two
   integers *)
begin
```

```
    if m<n then min:= m
    else min:= n;
end;

procedure bubble_sort(var list: ptr_to_corporation);
(* the following procedure sorts a list of corporations in
a linked list *)
var
   k, flag, j: integer;
   elements: arraytype;
   i: integer;
   temp: ptr_to_corporation;
begin
   flag:= num_corp;
   for i:= 1 to num_corp do
   begin
        elements[i]:= list;
        list:= list^.next;
   end;
   k:= num_corp;
   while flag>1 do
   begin
        k:= flag-1;
        flag:= 0;
        for j:= 1 to k do
             if elements[j]^.name>elements[j+1]^.name then
             begin
                  temp:= elements[j];
                  elements[j]:= elements[j+1];
                  elements[j+1]:= temp;
                  flag:= j;
             end;
   end;
   front:= elements[1];
   for i:= 1 to num_corp-1 do
        elements[i]^.next:= elements[i+1];
   new(temp);
   elements[num_corp]^.next:= temp;
   temp^.next:= nil;
end; (* of bubble sort *)

function binary_search(list: arraytype; name: corporation):integer;
(* the following function performs a binary search for a
given corporation *)
var
   k,m: integer;
   j: integer;
   found: boolean;
   count: integer;
begin
   count:= 0;
   found:= false;
   k:= 1;
   m:= num_corp;
```

```
   if name.name='A' then a_count:= a_count + 1;
   while (k<=m) and (not found) do
   begin
        j:= trunc((k+m)/2);
        if name.name=list[j]^.name then found:= true;
        if name.name<list[j]^.name then m:= j-1
        else k:= j+1;
        count:= count + 1;
   end;
   j:= 0;
   binary_search:= count;
end;

procedure strategy_1;
(* the exhaustive linear search technique *)
begin
   y:= 0;
   variance:= 0;
   for i:= 1 to m do var_count[i]:= 0;
   dummy:= nil;
   count:= 0;
   a_count:= 0;
   print_list(front);
   while count<=num_accesses do
   begin
        corp_oration:= next_record;
        k:= linear_search(corp_oration, dummy);
        y:= y+k;
        count:= count+1;
        writeln('z= ',y/count);
        if count<=m then var_count[count]:= k;
   end;
   mean:= y/num_accesses;
   writeln('The estimated mean of strategy #1 is ',mean:12:1,
       ' after ', num_accesses:9,' records.');
   for i:= 1 to m do variance:= variance +sqr(var_count[i]-mean);
   variance:= variance/(m-1);
   writeln('The estimated variance of strategy #1 is ',variance:9:6,
       ' after ',num_accesses:9,' records.');
   writeln('The access probability of corporation A with strategy
       #1 is ',a_count/num_accesses:8:6,' after ',num_accesses:9,
       ' records.');
end; (* of strategy_1 *)

procedure strategy_2;
(* the head of line technique *)
y:= 0;
variance:= 0;
for i:= 1 to m do var_count[i]:= 0;
dummy:= nil;
count:= 0;
a_count:= 0;
print_list(front);
while count<= num_accesses do
```

```
begin
   corp_oration:= next_record;
   k:= search_and_move(corp_oration);
   y:= y+k;
   count:= count+1;
   mean:= y/count;
   if count<=m then var_count[count]:= k;
end;
mean:= y/num_accesses;
   writeln('The estimated mean of strategy #2 is ',mean:12:1,
       ' after ', num_accesses:9,' records.');
   for i:= 1 to m do variance:= variance +sqr(var_count[i]-mean);
   variance:= variance/(m-1);
   writeln('The estimated variance of strategy #2 is ',variance:9:6,
       ' after ',num_accesses:9,' records.');
   writeln('The access probability of corporation A with strategy
       #2 is ',a_count/num_accesses:8:6,' after ',num_accesses:9,
       ' records.');
end; (* of strategy_2 *)


procedure strategy_3;
(* the swap forward one position technique *)
begin
   y:= 0;
   for i:= 1 to m do var_count[i]:= 0;
   variance:= 0;
   dummy:= nil;
   count:= 0;
   a_count:= 0;
   print_list(front);
   while count<= num_accesses do
   begin
        corp_oration:= next_record;
        k:= search_and_swap(corp_oration);
        y:= y+k;
        count:= count+1;
        mean:= y/count;
        if count<=m then var_count[count]:= k;
   end;
   mean:= y/num_accesses;
   writeln('The estimated mean of strategy #3 is ',mean:12:1,
       ' after ', num_accesses:9,' records.');
   for i:= 1 to m do variance:= variance +sqr(var_count[i]-mean);
   variance:= variance/(m-1);
   writeln('The estimated variance of strategy #3 is ',variance:9:6,
       ' after ',num_accesses:9,' records.');
   writeln('The access probability of corporation A with strategy
       #3 is ',a_count/num_accesses:8:6,' after ',num_accesses:9,
       ' records.');
end; (* of strategy_3 *)


procedure strategy_4(l: ptr_to_corporation);
```

```
  (* the optimum technique: binary search *)
  var
     i: integer;
     elements: arraytype;
  begin
     y:= 0;
     for i:= 1 to m do var_count[i]:= 0;
     variance:= 0;
     dummy:= nil;
     count:= 0;
     a_count:= 0;
     print_list(front);
     for i:= 1 to num_corp do
     begin
          elements[i]:= l;
          l:= l^.next;
     end;
     while count<=num_accesses do
     begin
          corp_oration:= next_record;
          k:= binary_search(elements, corp_oration);
          y:= y+k;
          count:= count+1;
          mean:= y/count;
          if count<=m then var_count[count]:= k;
     end;
     mean:= y/num_accesses;
     writeln('The estimated mean of strategy #4 is ',mean:12:1,
         ' after ', num_accesses:9,' records.');
     for i:= 1 to m do variance:= variance +sqr(var_count[i]-mean);
     variance:= variance/(m-1);
     writeln('The estimated variance of strategy #4 is ',variance:9:6,
         ' after ',num_accesses:9,' records.');
     writeln('The access probability of corporation A with strategy
         #4 is ',a_count/num_accesses:8:6,' after ',num_accesses:9,
         ' records.');
  end; (* of strategy_4 *)

begin (* of main_body *)
     m:= min(num_accesses, max_variance_samples);
     strategy_1;
     put_seed(7774755);
     strategy_2;
     put_seed(7774755);
     strategy_3;
     put_seed(7774755);
     bubble_sort(front);
     strategy_4(front);
     put_seed(7774755);
end; (* of main_body *)

begin
     initialize;
     main_body;
```

```
end.
```

The extra overhead involved in the binary search includes, consuming much memory for large n, the extra $\bigcirc(n)$ operations needed to copy the list into the array.

Let the iid sequence be the numbers generated by **x_random.** Then $x_i \sim U(0,1)$. $E(x_i) = \frac{0+1}{2} = 0.5$.

$\hat{\mu} = 5.2$, $\sigma^2 = 13.57$. Let $x_1, x_2, ...$ be the measurements

$$\frac{s_n}{n} = \frac{1}{n}\sum_{i=1}^{n} x_i.$$

Let μ be the true mean and σ^2 the true variance.

$$\mu - 0.05\mu < \frac{s_n}{n} < \mu + 0.05\mu.$$

$$P\left(\mu - 0.05\mu < \frac{s_n}{n} < \mu + 0.05\mu\right) > 0.95.$$

The Central Limit Theorem says

$$w_n = \frac{\frac{s_n}{n} - \mu}{\frac{\sigma}{\sqrt{n}}} \to z,$$

in distribution, $z \sim N(0,1)$. Then, $w_n \sim N(0,1)$. And,

$$\frac{\frac{s_n}{n} - \hat{\mu}}{\frac{\hat{\sigma}}{\sqrt{n}}} \to z,$$

So,

$$P\left(\frac{-0.05\hat{\mu}}{\frac{\hat{\sigma}}{\sqrt{n}}} < \frac{\frac{s_n}{n} - \hat{\mu}}{\frac{\hat{\sigma}}{\sqrt{n}}} < \frac{0.05\hat{\mu}}{\frac{\hat{\sigma}}{\sqrt{n}}}\right) > 0.95 \Rightarrow P\left(\frac{-0.05\hat{\mu}}{\frac{\hat{\sigma}}{\sqrt{n}}} < Z < \frac{0.05\hat{\mu}}{\frac{\hat{\sigma}}{\sqrt{n}}}\right) > 0.95 \Rightarrow$$

$$P\left(\frac{-0.05(5.2)}{\frac{3.68}{\sqrt{n}}} < Z < \frac{0.05(5.2)}{\frac{3.68}{\sqrt{n}}}\right) > 0.95 \Rightarrow 2\Phi\left(\frac{0.26\sqrt{n}}{3.68}\right) - 1 > 0.95 \Rightarrow \frac{0.26\sqrt{n}}{3.68} > 1.96 \Rightarrow n > 769.6.$$

We used approximations of μ and σ^2 to obtain n.

To use the Central Limit Theorem, an iid sequence of measurements is needed. The number of references to nodes in the list are only independent in the linear search technique. Other than assuming that a given corporation does reside somewhere in the list, no rearrangement to the list took place. The other three techniques rearranged the list. By rearranging the list, the measurements have been altered to minimize the number of nodes being reference. Other approximations used besides $\hat{\mu}$ are $\hat{\sigma}$ for each technique. We assume that the measurements in the linear search are identically distributed. We also assumed the pseudo random number generator would generate random input instances for an infinite number of calls when in reality the pseudo random number generator will repeat sequences of input instances after a finite number of calls. So actually, we do not have random variables in this program by the definition of a random variable.

An example of a sample run which almost surely converges to 5 is $w = (5, 5, 5, ..., 5, ...)$. An example of a sample run on which the sequence does not converge to 5 is $w' = (1, 1, 1, ..., 1, ...)$.

To answer the last question, the distribution is Geometric. The same standard calculations are used.

4.36 Markov Terminology

A *stochastic process* is a collection of random variables such that $\{x_s, s \in I\}$, I is the index set and R is the state space or range for each x_s. The *index set* can be 1) countable and finite (discrete), or 2) uncountable(continuous). The *state space* can be countable and finite, or 2) uncountable. There are 4 types of stochastic processes:

1. discrete time, discrete state space - iid Bernoulli.
2. discrete time, continuous state space - iid Uniform.
3. continuous time, discrete state space - # of programs executing at time s.
4. continuous time, continuous state space.

4.36.1 Markov Chains

Example: A strange board game, $\{A, B, C, D, E\}$. See the Figure 4.1.

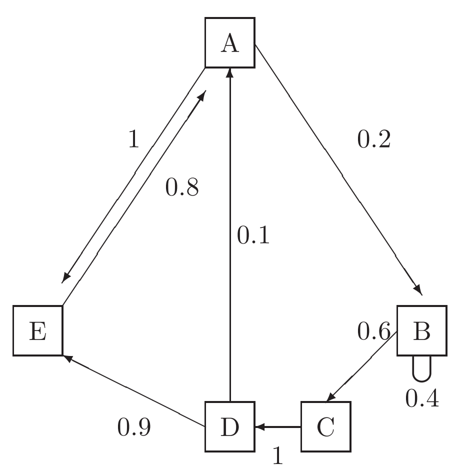


Figure 4.1: Strange Board Game

Let V_1 be the first random number such, $I_{AB}(0.2) + I_{AE}(0.8) = 1$. x_1 is the square after the first jump. x_2 is the square after the second jump. x_3 is the square after the third jump, and so on. $\{x_n : n = 1, 2, 3, ...\}$

$R_{x_n} = \{A, B, C, D, E\}$ is the state space. $I = \{1, 2, 3, ...\}$.

$$P(x_4 = E | x_0 = A, x_1 = B, x_2 = C, x_3 = D) = \frac{P(x_0 = A, x_1 = B, x_2 = C, x_3 = D, x_4 = E)}{P(x_0 = A, x_1 = B, x_2 = C, x_3 = D)} =$$

$$\frac{P(V_1 \in I_{AB}, V_2 \in I_{BC}, V_3 \in I_{CD}, V_4 \in I_{DE})}{P(V_1 \in I_{AB}, V_2 \in I_{BC}, V_3 \in I_{CD})} = \frac{P(V_1 \in I_{AB})P(V_2 \in I_{BC})P(V_3 \in I_{CD})P(V_4 \in I_{DE})}{P(V_1 \in I_{AB})P(V_2 \in I_{BC})P(V_3 \in I_{CD})} =$$

$$P(V_4 \in I_{DE}).$$

But, $P(x_4 = E | x_3 = D) = P(V_4 \in I_{DE})$.

A *Markov chain* is a stochastic process $\{x_n\}$ with index set $I = \{1, 2, 3, ...\}$ and counts the state space R_x such that for all $n \in I$ and $k_i \in R_x$:

$$P(x_{n+1} = k_{n+1} | x_0 = k_0, x_1 = k_1, ..., x_n = k_n) = P(x_{n+1} = k_{n+1} | x_n = k_n).$$

A Markov chain is *time homogeneous* if for all n,

$$P(x_{n+1} = k_{n+1} | x_n = k_n) = P(x_1 = k_{n+1} | x_0 = k_n).$$

Example: Consider a data structure in which items are added or deleted, with each access to the list structure. The probability that an access is an addition is p, independent of any other accesses. Let x_0 be the initial number of items. Let x_n be the number of items after the n-th access. $\{x_0, x_1, x_2, ...\}$ is a stochastic process. The state space is $R_{x_n} = \{0, 1, 2, 3, ...\}$. The state diagram is appears in Figure 4.2.

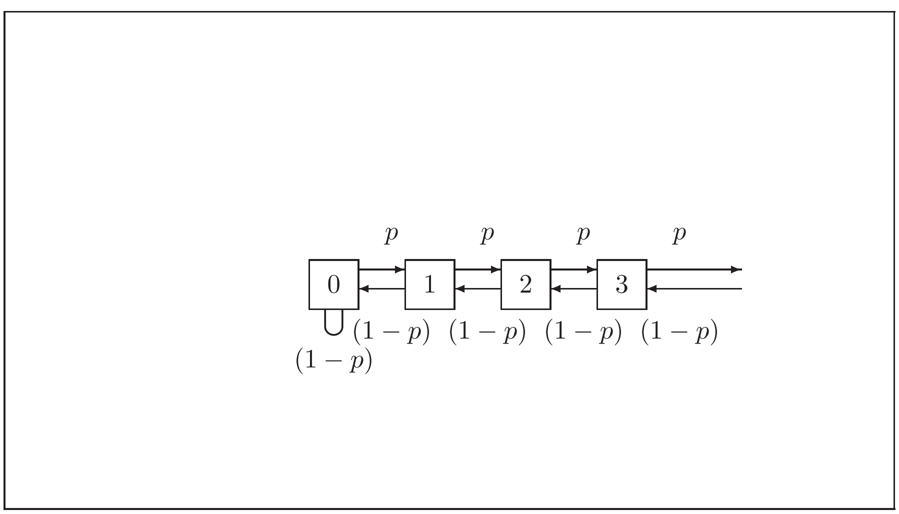


Figure 4.2: A Markov Chain

Is the Markov definition satisfied?

$$P(x_{n+1} = k_{n+1} | x_0 = k_0, x_1 = k_1, ..., x_n = k_n) = \begin{cases} p, & \text{if } k_{n+1} = k_n + 1. \\ 1 - p, & \text{if } k_{n+1} = k_n - 1. \end{cases}$$

4.36.2 Transition Matrix

Let $\mathrm{IP}_{ij} = P(x_{n+1} = j | x_n = i)$. The transition matrix is given by $\mathrm{IP} = [\mathrm{IP}_{ij}]$.

Example: Consider the state diagram in Figure 4.3.

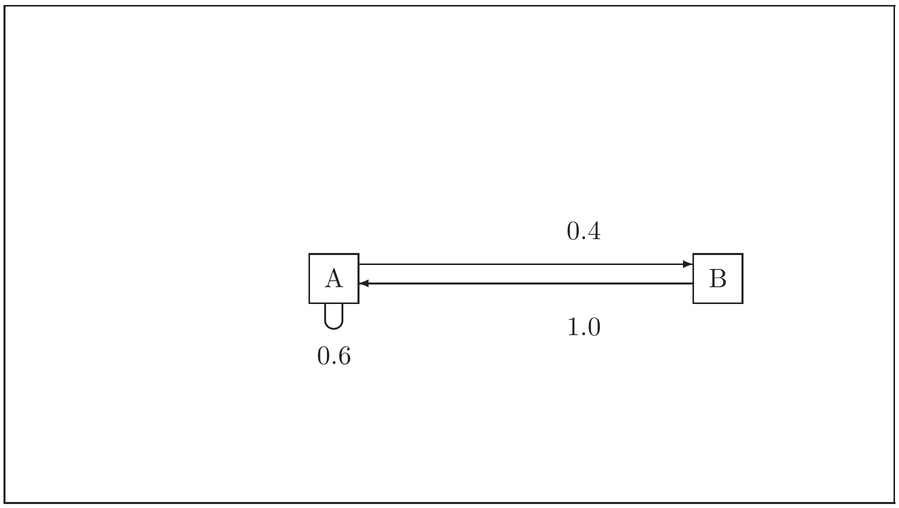


Figure 4.3: A Non-State Diagram

Renumber the states as in Figure 4.4.

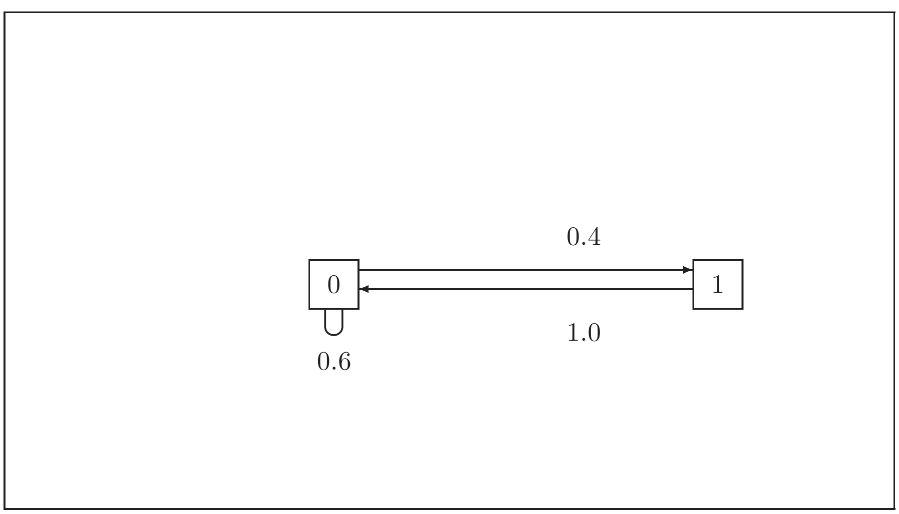


Figure 4.4: The Fixed State Diagram

$\mathrm{IP}_{00} = 0.6, \mathrm{IP}_{10} = 1.0, \mathrm{IP}_{01} = 0.4, \mathrm{IP}_{11} = 0$. Then, the transition matrix is stated as:

$$\mathrm{IP} = \begin{vmatrix} 0.6 & 0.4 \\ 1 & 0 \end{vmatrix}$$

Example: The data structure example. $\mathrm{IP}_{00} = 1-p$, $\mathrm{IP}_{01} = p$, $\mathrm{IP}_{10} = 1-p$, $\mathrm{IP}_{11} = 0$.

$$\begin{array}{c|cccccc|} & 0 & 1 & 2 & 3 & & \\ 0 & 1-p & p & 0 & 0 & 0 & \ldots \\ 1 & 1-p & 0 & p & 0 & 0 & \ldots \\ 2 & 0 & 1-p & 0 & p & 0 & \ldots \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \end{array}$$

For any Markov chain,

$$P(x_i = j, x_0 = i) = P(x_i = j | x_0 = i) P(x_0 = i).$$

$$P(x_2 = k, x_1 = j, x_0 = i) = P(x_2 = k | x_1 = j, x_0 = i) P(x_1 = j, x_0 = i) =$$
$$P(x_2 = k | x_1 = j) P(x_1 = j | x_0 = i) P(x_0 = i).$$

Example:

$$\mathrm{IP} = \begin{vmatrix} 0.6 & 0.4 \\ 1 & 0 \end{vmatrix}$$

$$\mathrm{IP}_{ij}^{(1)} = P(x_1 = j | x_0 = i) = P(x_n = j | x_{n-1} = i) = P(x_2 = k | x_0 = i) =$$

$$\frac{P(x_2 = k, x_0 = i)}{P(x_0 = i)} = \sum_j \frac{P(x_2 = k, x_1 = j, x_0 = i)}{P(x_0 = i)} =$$

$$\frac{\sum_j P(x_2 = k | x_1 = j) P(x_1 = j | x_0 = i) P(x_0 = i)}{P(x_0 = i)} = \sum_j P(x_2 = k | x_1 = j) P(x_1 = j | x_0 = i) = \sum_j P_{jk}^{(1)} P_{ij}^{(1)}.$$

$$P_{01}^{(2)} = \sum_{j=0,1} P_{0j}^{(1)} P_{j1}^{(1)} = P_{00}^{(1)} P_{01}^{(1)} + P_{01}^{(1)} P_{11}^{(1)} = 0.6(0.4) + 0.4(0) = 0.24.$$

$$P_{00}^{(2)} = \sum_j P_{0j}^{(1)} P_{j0}^{(1)} = P_{00}^{(1)} P_{00}^{(1)} + P_{01}^{(1)} P_{10}^{(1)} = 0.76.$$

$$\mathrm{IP}^2 = \begin{vmatrix} 0.6 & 0.4 \\ 1 & 0 \end{vmatrix} \qquad \begin{vmatrix} 0.6 & 0.4 \\ 1 & 0 \end{vmatrix} = \begin{vmatrix} 0.76 & 0.24 \\ 0.6 & 0.4 \end{vmatrix}$$

Thus, $\mathrm{IP}^{(2)} = \mathrm{IP}^2$. In general, $\mathrm{IP}^{(n)} = \mathrm{IP}^n$.

$$\mathrm{IP}^{(3)} = \begin{vmatrix} 0.696 & 0.504 \\ 0.76 & 0.24 \end{vmatrix}, \ \mathrm{IP}^{(4)} = \begin{vmatrix} 0.721 & 0.278 \\ 0.696 & 0.304 \end{vmatrix}, \ \mathrm{IP}^{(5)} = \begin{vmatrix} 0.711 & 0.288 \\ 0.721 & 0.278 \end{vmatrix}, \ \ldots \mathrm{IP}^{(50)} = \begin{vmatrix} 0.714 & 0.285 \\ 0.714 & 0.285 \end{vmatrix}$$

$\mathrm{IP}^{(1)}, \mathrm{IP}^{(2)}, \mathrm{IP}^{(3)}, \ldots$ is a sequence. If $\mathrm{IP}^{(n)} \to L$, then $\mathrm{IP}_{ij}^{(n)} \to L_j = \prod_j$.

$$\mathrm{IP}_{ij}^{(n)} = \sum_k \mathrm{IP}_{ik}^{(n-1)} \mathrm{IP}_{kj}^{(1)}, \ \Pi_j = \sum_k \Pi_k \mathrm{IP}_{kj}, \ \Pi_0 = \Pi_0 \mathrm{IP}_{00} + \Pi_1 \mathrm{IP}_{10} = \frac{1}{1.4}, \ \Pi_1 = \frac{0.4}{1.4}.$$

The rows sum to 1. $\sum_j \Pi_j = 1$.

Example: See the state diagram in Figure 4.5.

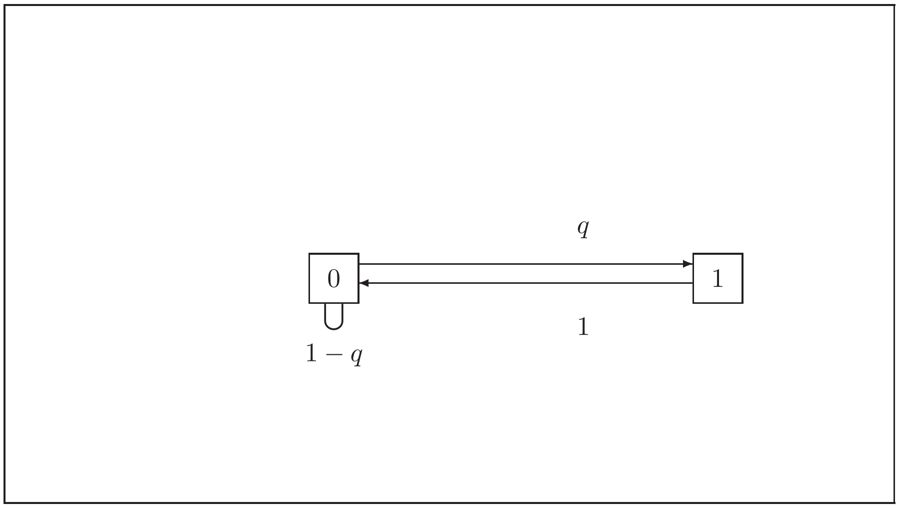


Figure 4.5: A State Diagram

$$\mathrm{IP} = \begin{vmatrix} 1-q & q \\ 1 & 0 \end{vmatrix}$$

Use $\Pi_j = \sum_k \Pi_k \mathrm{IP}_{kj} = 1$.

$$\Pi_0 = \Pi_0 \mathrm{IP}_{00} + \Pi_1 \mathrm{IP}_{10} = \Pi_0(1-q) + \Pi_1.$$

$$\Pi_1 = \Pi_0 \mathrm{IP}_{01} + \Pi_1 \mathrm{IP}_{11} = \Pi_0 q + 0.$$

$$\Pi_0 + \Pi_1 = 1.$$

Solve the above three equations simultaneously.

$$\Pi_1 = \Pi_0 q$$

$$\Pi_0 + \Pi_0 q = 1 \Rightarrow \Pi_0 = \frac{1}{1+q}.$$

$$\Pi_1 = 1 - \Pi_0 = 1 - \frac{1}{1+q} = \frac{q}{1+q}.$$

$\Pi = (\Pi_0 \Pi_1)$.

$$(\Pi_0 \Pi_1) = (\Pi_0 \Pi_1) \begin{vmatrix} 1-q & q \\ 1 & 0 \end{vmatrix}.$$

Or use $\Pi = \Pi \mathrm{IP}$. The steady state equations are derived from $\sum_j \Pi_j = 1$. The steady state distribution is given by:

$$\mathrm{IP}_{ij}^{(n)} \to \Pi_j,\ \mathrm{IP}_{0j}^{(n)} \to \Pi_j,\ \mathrm{IP}_{1j}^{(n)} \to \Pi_j,\ \ldots$$

Example: Consider the state diagram in Figure 4.6:

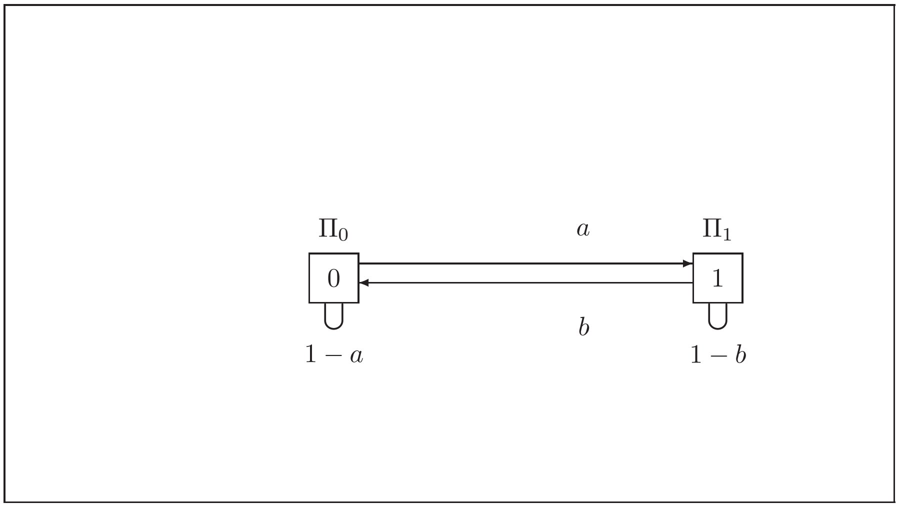


Figure 4.6: A State Diagram

The steady state equations are derived from, $\Pi = \Pi\mathrm{P}$, and $\sum_j \Pi_j = 1$.

$$\Pi_0 = \Pi_0(1-a) + \Pi_1 b. \tag{4.1}$$

$$\Pi_1 = |\Pi_1(1-b) + \Pi_0 a. \tag{4.2}$$

$$\Pi_0 + \Pi_1 = 1. \tag{4.3}$$

Solve the above 3 equations simultaneously to obtain $\Pi_0 = \frac{b}{a+b}$, $\Pi_1 = \frac{a}{a+b}$.

$$P(x_n = 0) = \sum_j P(x_n = 0|x_0 = j)P(x_0 = j) \cong \sum_j \Pi_0 P(x_0 = j) = \Pi_0 \sum_j P(x_0 = j) = \Pi_0.$$

$$P(x_n = 0) \to \Pi_0,$$

or

$$P(x_n = i) \to \Pi_i.$$

For an n-state Markov chain,

$$\sum_{j=0}^{n} \Pi_j = 1.$$

$(\Pi_0, \Pi_1, ..., \Pi_k)$ is a pmf of some random variable N. $P(N = i) = \Pi_i, i = 0, 1, ..., k$. $x_n \to N$ in distribution. $E(N) = \sum_j jP(N = j) = \sum_j j\Pi_j$. $E(x_n) \cong E(N)$.

Example: Consider the data structure example again.

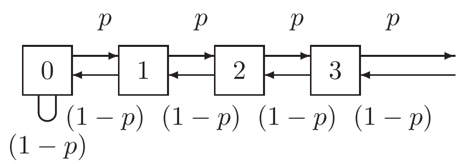


Figure 4.7: A Data Structure

Additions to the list occur with probability p. Deletions occur with probability $1-p$. Let x_n be the number of items in the structure after the n-th access. The steady state equations are derived as follow:

$$\Pi_0 = \Pi_0(1-p) + \Pi_1(1-p),$$

$$\Pi_1 = \Pi_0 p + \Pi_2(1-p),$$
$$\Pi_2 = \Pi_1 p + \Pi_3(1-p),$$
$$\Pi_3 = \Pi_2 p + \Pi_4(1-p),$$
$$...$$
$$\Pi_0 + \Pi_1 + \cdots = 1.$$

Solve for Π :

$$\Pi_k = \Pi_{k-1}p + \Pi_{k+1}(1-p).$$

Write as,

$$\Pi_k(1-p+p) = \Pi_{k-1}p + \Pi_{k+1}(1-p).$$

Then,

$$\Pi_k(1-p) + \Pi_k p = \Pi_{k-1}p + \Pi_{k+1}(1-p) = \overbrace{\Pi_{k+1}(1-p) - \Pi_k p}^{g_k} = \overbrace{\Pi_k(1-p) - \Pi_{k-1}p}^{g_{k-1}},$$

$g_k = g_{k-1}$. Therefore, $g_k = g_{k-1} = g_{k-2} = ... = g_1$. Then going back to the first equation,

$$\Pi_0 = \Pi_0(1-p) + \Pi_1(1-p) = \Pi_0 - \Pi_0 p + \Pi_1(1-p),$$

Then,

$$\Pi_1(1-p) - \Pi_0 p = 0 (g_1 = 0).$$

Then, $g_k = 0$. So,

$$\Pi_{k+1}(1-p) - \Pi_k p = 0,$$

$$\Pi_1 = \frac{p}{1-p}\Pi_0.$$

$$\Pi_2 = \frac{p}{1-p}\Pi_1 = \left(\frac{p}{1-p}\right)^2 \Pi_0.$$

$$\Pi_3 = \left(\frac{p}{1-p}\right)^3 \Pi_0.$$

...

$$\Pi_k = \left(\frac{p}{1-p}\right)^k \Pi_0.$$

Then we have

$$\Pi_0 + \frac{p}{1-p}\Pi_0 + \left(\frac{p}{1-p}\right)^2 \Pi_0 + \cdots = 1,$$

$$\Pi_0(1 + x + x^2 + \cdots) = 1,$$

when $x = \frac{p}{1-p}$.

$$\Pi_0 = 1 - x = 1 - \frac{p}{1-p} = \frac{1-2p}{1-p}.$$

Therefore,

$$\left(\frac{p}{1-p}\right)^k \Pi_0 = \left(\frac{p}{1-p}\right)\left(\frac{1-2p}{1-p}\right).$$

$|x| < 1$, $\frac{p}{1-p} < 1$. Thus a steady state condition is $p < \frac{1}{2}$.

Let N be a random variable with pmf Π. $P(N = k) = \Pi_k$. $x_n \to N$ in distribution.

$$E(N) = \sum kP(N = k) = \sum_{k=0}^{\infty} k\Pi_k = \sum_{k=0}^{\infty} k \left(\frac{p}{1-p}\right)^k \left(\frac{1-2p}{1-p}\right) = \frac{p}{1-2p}.$$

$$E(x_n) \cong \frac{p}{1-2p}.$$

4.36.3 Existence of Steady State Solutions

For finite state space Markov chains, steady state solutions do not always exist. Consider the state diagram in Figure 4.8:

$$\mathrm{IP} = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}$$

$\Pi_0 = \Pi_1$, $\Pi_1 = \Pi_0$, $\Pi_0 + \Pi_1 = 1$. Thus, $\Pi_0 = \Pi_1 = \frac{1}{2}$.

$$\mathrm{IP}^{(2)} = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \ \mathrm{IP}^{(3)} = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}$$

$\mathrm{IP}^{(n)}$ does not converge to anything.

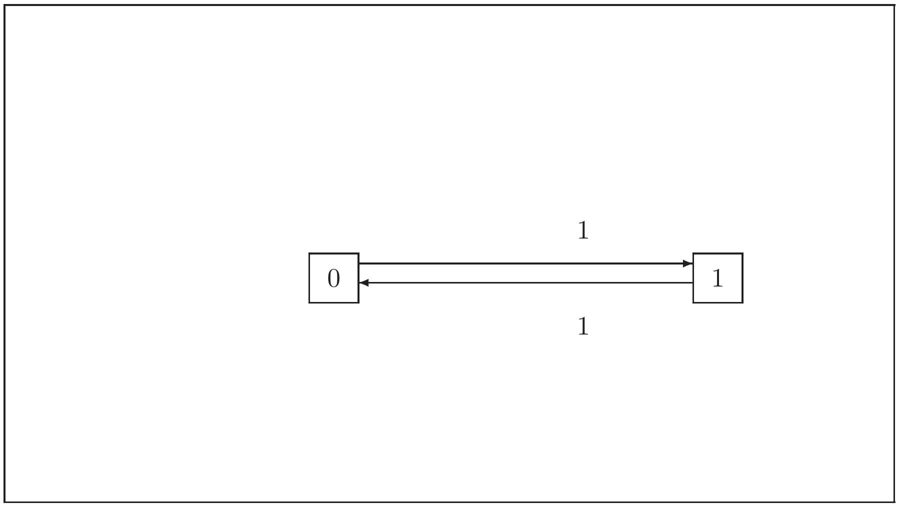


Figure 4.8: A State Diagram

4.36.4 More Markov Chain Terminology

Consider only finite state spaces.

- *Reachable* - state j is reachable from i, $i \to j$, if $\mathrm{IP}_{ij}^{(n)} > 0$ for some $n \geq 1$.
- *Communicate* - state i communicates with state j if $i \to j$ and $j \to i$, which is the same as $i \leftrightarrow j$.
- *Irreducible* - A Markov chain in which all states communicate with all other states is called Irreducible.
- *Periodicy* - $H(i) = \{j \in R_x, \mathrm{IP}_{ij} > 0\}$ Define for state i

$$A_i^{(1)} = H(i),\ A_i^{(2)} = \bigcup_{j \in A} H(j),\ \dots\ A_i^{(n)} = \bigcup_{j \in A_i^{(n-1)}} H(j).$$

An Irreducible Markov chain(with a finite state space) is *aperiodic* if there exists m such that $\forall n > m$, $A_i^{(n)} = R_x$, for every i.

Example: Consider the state diagram in Figure 4.9 again:

$H(0) = \{1\}$, $H(1) = \{0\}$. At $i = 0$, $A_0^{(1)} = H(0) = \{1\}$, $A_0^{(2)} = \bigcup_{j \in A_0^{(1)}} H(j) = H(0) = \{0\}$.

Example: Consider the state diagram in Figure 4.10:

$H(0) = \{0, 1\}$, $H(1) = \{1\}$. For $i = 0$: $A_0^{(1)} = \{0, 1\}$, $A_0^{(2)} = \{0, 1\}$, ... $A_0^{(n)} = \{0, 1\}$. For $i = 1$: $A_1^{(1)} = \{0\}$, $A_1^{(2)} = \{0, 1\}$, ...

The main result is this: let IP be the transition matrix of a finite, aperiodic, Irreducible Markov chain with state space $\{0, 1, ..., k\}$. Then there exists a vector $\Pi = (\Pi_0, \Pi_1, ..., \Pi_k)$ such that:

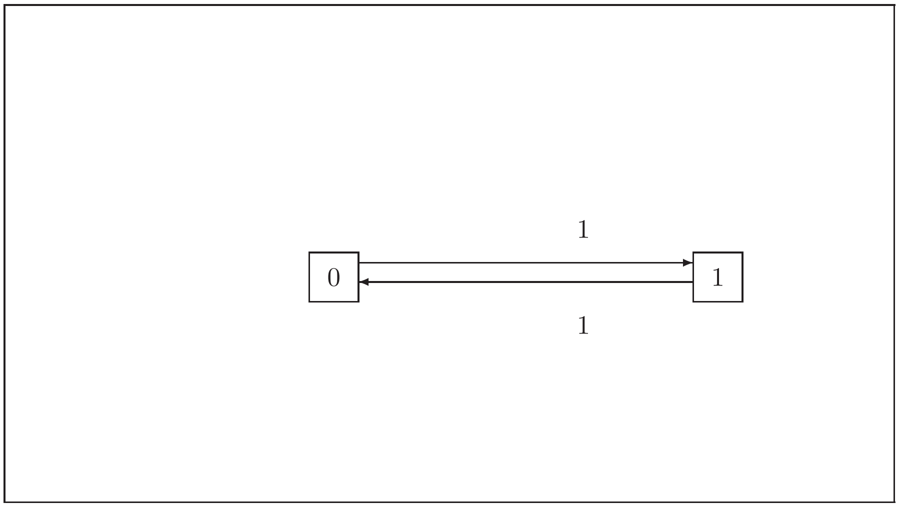


Figure 4.9: A State Diagram

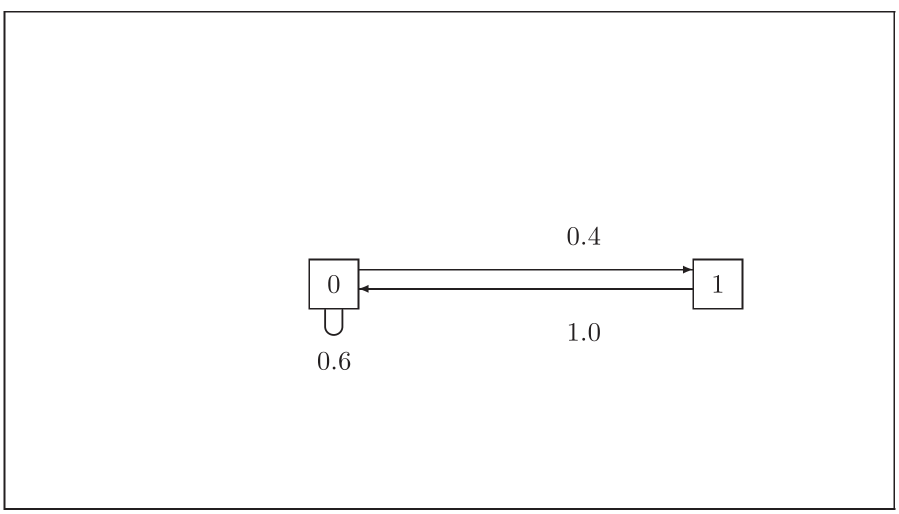


Figure 4.10: A State Diagram

1. $\mathrm{IP}_{ij}^{(n)} \to \Pi_j$.
2. Π is the only solution to $\Pi_k = \Pi \mathrm{IP}$, $\sum_{i=0}^{\infty} \Pi_i = 1$.

4.36.5 Theory of Markov Chains

Consider infinite state spaces, irreducibility, and transient behavior. See the state diagram in Figure 4.11:

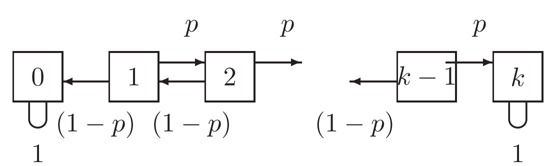


Figure 4.11: A State Diagram

The diagram is considered to be a random walk. $\{0, 1\}$ are called absorbing states. The random walk is also called the *gambler's ruin*.

4.36.6 Continuous Time, Discrete State Space Stochastic Model

$x_s \in \{0, 1, 2, ...\}$, $s \in \Re^+$.

$$P(x_s = q_s | x_v = q_u, 0 \le u \le v < s) = P(x_s = q_s | x_v = q_u),$$

or,

$$P(x_{s_k} = q_k | x_{s_1} = q_1, ..., x_{s_{k-1}} = q_{k-1}) = P(x_{s_k} = q_k | x_{s_{k-1}} = q_{k-1}), 0 \le s_1 \le s_2 \le \cdots \le s_k.$$

Time spent in one state is exponentially distributed as opposed to Geometrically distributed.

4.36.7 Poisson Process

The Poisson distribution is stated as follow: $x \sim Poisson(\lambda)$,

$$P(x = k) = \frac{\lambda^k e^{-\lambda}}{k!}, k = 0, 1, 2, ...$$

To approximate the Binomial distribution with the Poisson distribution, let $\lambda = np$. The approximation is good when n is large and p is small.

$$P(x = k) = \frac{\lambda^k e^{-\lambda}}{k!} =$$

$$\left(\begin{array}{c} n \\ k \end{array}\right) p^k(1-p)^{n-k} = \frac{n!p^k(1-p)^{-k}(1-p)^n}{k!(n-k)!} \cong \frac{1}{k!}n^k p^k (1-p)^{-k}(1-p)^n = \frac{1}{k!}\lambda^k (1-p)^{-k}(1-p)^n \to \frac{\lambda^k e^{\lambda}}{k!}.$$

In a Poisson process, N_s is the number of arrivals in the interval $[0, s]$. Postulates:

1. Non-overlapping intervals are independent. If $[s_1, s_2], [s_3, s_4]$ are independent, then so are $N_{s_2} - N_{s_1}$ and $N_{s_4} - N_{s_3}$.

2. $$\frac{P(\text{exactly 1 arrival in } [s, s+\triangle s])}{\triangle s} \to \lambda,$$

   as $\triangle s \to 0$.

3. $$\frac{P(\text{more than 1 arrival in } [s, s+\triangle s])}{\triangle s} \to 0,$$

   as $\triangle s \to 0$.

$$P(N_s = k) = \frac{(\lambda s)^k e^{-\lambda s}}{k!}, \ \ N_s \sim Poisson(\lambda s), \ \ E(N_s) = \lambda s. x_1, x_2, x_3, ...,$$

$$P(x_1 > s) = P(\text{no arrivals in } [0, s]) = P(N_s = 0) = \frac{\lambda s^0 e^{-\lambda s}}{0!} = e^{-\lambda s}.$$

Therefore, $P(x_1 = s) = 1 - e^{-\lambda s}$, $x_1 \sim Exp(\lambda)$.

4.37 Homework and Answers

1. Suppose $X \sim Binomial(n, Y)$ where Y is itself a random variable with pmf:

   $$P\left(Y = \frac{1}{4}\right) = \frac{1}{4}, \ \ P\left(Y = \frac{1}{2}\right) = \frac{1}{2}, \ \ P\left(Y = \frac{3}{4}\right) = \frac{1}{4}.$$

   Compute $E(X)$ using conditional expectation. [Hint: Start by computing $E(X|Y = y)$].

   $$E(x) = \sum_k E(x|y = k)P(y = k) =$$

   $$E\left(x \middle| y = \frac{1}{4}\right) P\left(y = \frac{1}{4}\right) + E\left(x \middle| y = \frac{1}{2}\right) P\left(y = \frac{1}{2}\right) + E\left(x \middle| y = \frac{3}{4}\right) P\left(y = \frac{3}{4}\right).$$

   $$E(x|Y = y) = ny, \ \ E\left(x \middle| y = \frac{1}{4}\right) = \frac{n}{4}, \ \ E\left(x \middle| y = \frac{1}{2}\right) = \frac{n}{2}, \ \ E\left(x \middle| y = \frac{3}{4}\right) = \frac{3n}{4}.$$

   Then,

   $$E(x) = \frac{n}{4}\left(\frac{1}{4}\right) + \frac{n}{2}\left(\frac{1}{2}\right) + \frac{3n}{4}\left(\frac{1}{4}\right) = \frac{n}{2}.$$

2. Consider a Markov Chain X_n with the state transition diagram in Figure 4.12:

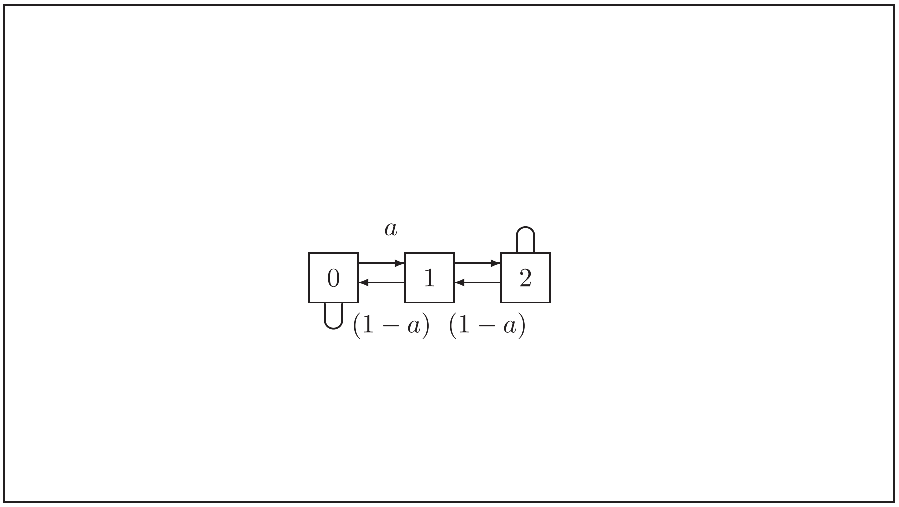


Figure 4.12: A Transition State Diagram

(a) Write down the state space and index set of the stochastic process X_n. The state space is $\{0, 1, 2\}$. The index set is $\{0, 1, 2, 3, 4, ...\}$.

(b) Fill in the missing jump probabilities in the state transition diagram in Figure 4.13.

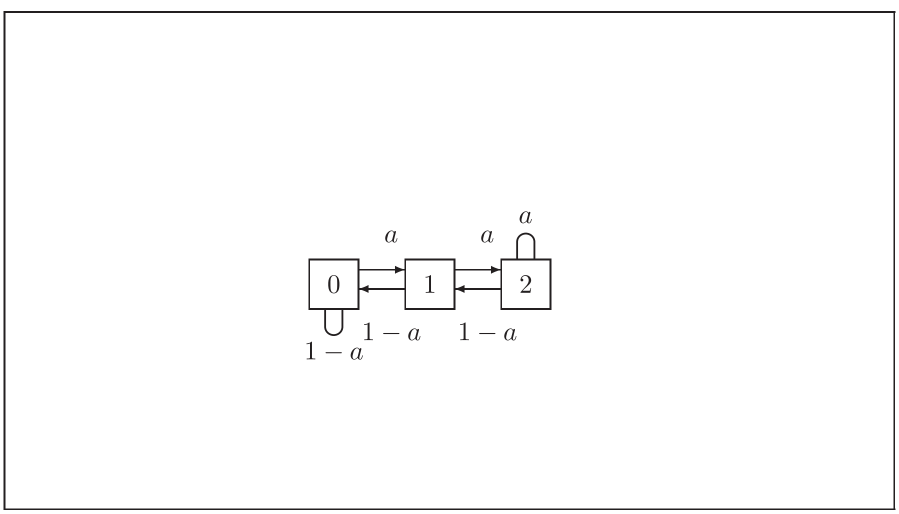


Figure 4.13:

(c) What is the transition matrix, IP, of the Markov chain?

$$\begin{vmatrix} 1-a & a & 0 \\ 1-a & 0 & a \\ 0 & 1-a & a \end{vmatrix}$$

(d) Show that the Markov chain is aperiodic. $H(i) = \{j \in \{0,1,2\}, \mathrm{IP}_{ij} > 0\}$. $H(0) = \{0,1\}$, $H(1) = \{0,2\}$, $H(2) = \{1,2\}$. For $i = 0 : A_0^{(1)} = H(0) = \{0,1\}$, $A_0^{(2)} = \{0,1,2\}$. For $i = 1$: $A_1^{(1)} = \{0,2\}$, $A_1^{(2)} = \{0,1,2\}$. For $i = 2 : A_2^{(1)} = \{1,2\}$, $A_2^{(2)} = \{0,1,2\}$. Let $m = 1$. Then, $\forall n > m, A_i^{(n)} = R_x$ for every i. $(n \geq 2)$.

(e) Write down the equations for the steady state(limiting) pmf Π and solve for Π in terms of a.

$$\Pi_0 = \Pi_0(1-a) + \Pi_1(1-a),$$

$$\Pi_1 = \Pi_0 a + \Pi_2(1-a),$$

$$\Pi_2 = \Pi_1 a + \Pi_2 a,$$

$$\Pi_0 + \Pi_1 + \Pi_2 = 1.$$

Solve the above four equations simultaneously.

(f) If N is a random variable with pmf Π(i.e. so that $X_n \to N$ in distribution), then compute $E(N)$ in terms of a.

$$E(N) = \sum_{k=0}^{2} kP(N=k) = \sum_{k=0}^{2} k\Pi_k = 0\Pi_0 + 1\Pi_1 + 2\Pi_2.$$

Substitute in the answers from the previous question to obtain $E(N)$.

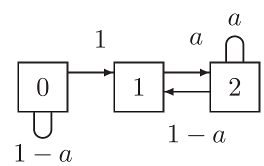
(g) Compute $\mathrm{IP}^{(2)}$ and $\mathrm{IP}^{(10)}$ when $a = 0.5$ and compare the results with Π. What do you observe? You may find it helpful to write a small program to do matrix multiplication.

$$\mathrm{IP}^{(1)} = \begin{vmatrix} 0.5 & 0.5 & 0 \\ 0.5 & 0 & 0.5 \\ 0 & 0.5 & 0.5 \end{vmatrix}, \ \mathrm{IP}^{(2)} = \begin{vmatrix} 0.5 & 0.25 & 0.25 \\ 0.25 & 0.5 & 0.25 \\ 0.25 & 0.25 & 0.5 \end{vmatrix}, \ \mathrm{IP}^{(10)} = \begin{vmatrix} 0.333 & 0.333 & 0.333 \\ 0.333 & 0.333 & 0.333 \\ 0.333 & 0.333 & 0.333 \end{vmatrix}$$

The probability matrix approaches those values of Π which are near steady state.

(h) Compute Π when $a = 0.25$ and when $a = 0.75$. Give an intuitive explanation for the resulting values of Π.

When $q = 0.25$, deletions to the list are more likely to occur. The pmf is bias towards the left side of the linked list. When $q = 0.75$, additions to the list are more likely to occur. The pmf is then bias towards the right side of the list.



(i) Remove an arc from the diagram in Figure 2i such that the resulting Markov chain is NOT Irreducible.

Not all states communicate. In the above case, states 0 and 1 do not communicate.

(j) Give an example of a 3-state Markov chain that is Irreducible, but not aperiodic. Show why your example is not aperiodic. When $a = 0$, or $a = 1$, the chain is Irreducible.

4.38 Final Exam and Answers

1. The continuous random variable X has a density function given by

$$f(x) = \begin{cases} cx, & \text{if } 0 < x < 10. \\ 0, & \text{otherwise.} \end{cases}$$

where $c = \frac{1}{50}$. Compute the variance of X.

$$Var(x) = \int (x-\mu)^2 f(x)\,dx = \int_0^{10} \frac{(x-\mu)^2}{50}\,dx = \frac{1}{50}\int_0^{10} (x^2 - 2x\mu + \mu^2)x\,dx =$$

$$\frac{1}{50}\int_0^{10} x^3 - 2x^2\mu + \mu^2\,dx = \frac{\frac{10^4}{4} - \frac{2(10)^3\mu}{3} + \frac{(10)^2\mu^2}{2}}{50}. \mu = E(x) = \int_{-\infty}^{\infty} xf(x)\,dx = \int_0^{10} \frac{x^2}{50}\,dx = 6.67.$$

Then,

$$Var(x) = \frac{\frac{10^4}{4} - \frac{2(10)^3 6.67}{3} + \frac{10^2(6.67)^2}{2}}{50} = \frac{277.78}{50}.$$

2. Consider an iid sequence $x_1, x_2, ...$ where the pmf of each x_i is given by $P(x_i = 2) = 0.6$, $P(x_i = 5) = 0.4$. Let $W_n = \frac{1}{n}\sum_{i=1}^{n} x_i$.

   (a) Does x_n converge almost surely to any limit? Explain. $x_n \to L$ almost surely if $P(x_n \to L) = 1$. x_n does not converge to any limit. The sequence of $x_1, x_2, x_3, ...$ just keeps repeating values 2 and 5 without converging.

(b) Does W_n converge almost surely to any limit? If so, what is that limit? $W_n \to L$ almost surely if

$$P\left(W : \frac{s_n(w)}{n} \to L\right) = 1.$$

$s_n(w) = \sum_{i=1}^{n} x_i$. $L = \mu = E(x_i)$. $E(x_i) = 2(0.6)+5(0.4) = 3.2$. Therefore, $P\left(W : \frac{s_n(w)}{n} \to 3.2\right) = 1$ by the Strong Law of Large Numbers.

(c) Give an example of a sample path on which W_n converges and one on which W_n does not converge. W_n converges on (2, 5, 2, 5, ...) to 3.5.

3. Consider the transition diagram in Figure 4.14 for a Markov chain $\{X_n\}$.

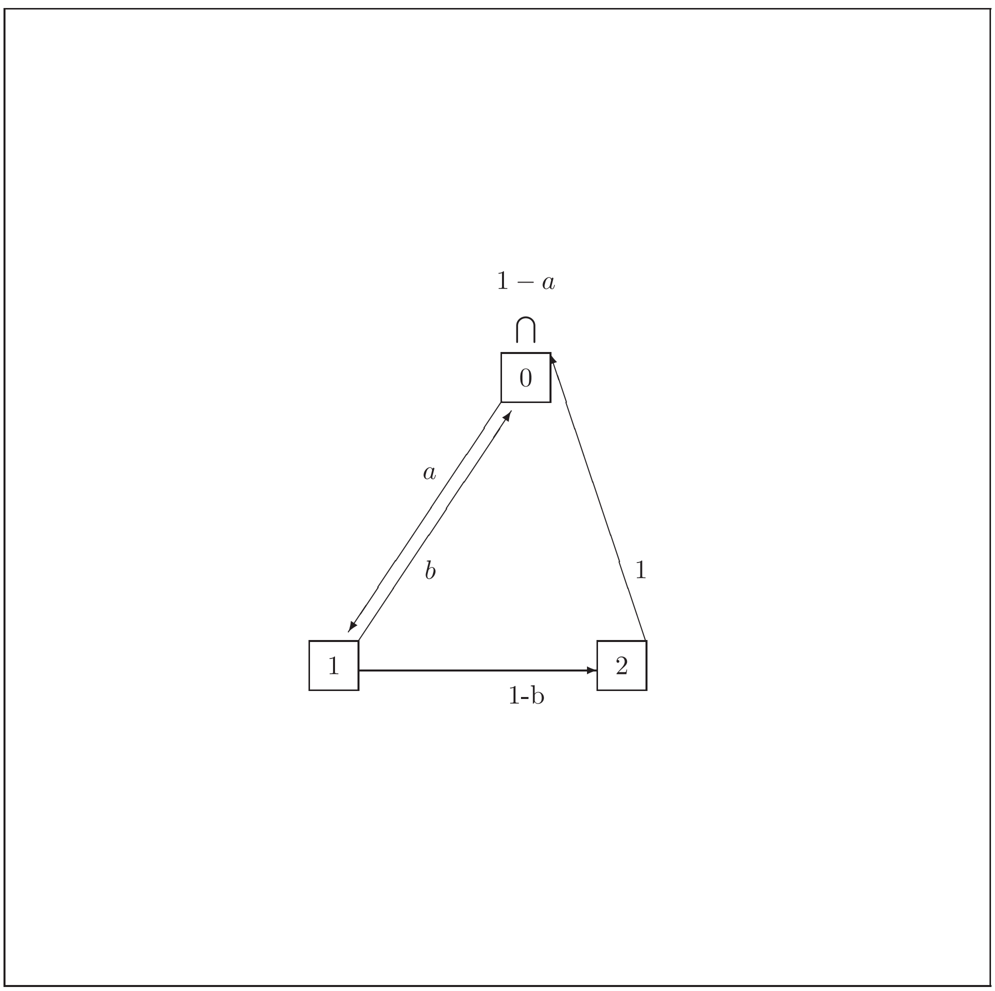


Figure 4.14:

(a) Show that the Markov chain is aperiodic.

For $i = 0 : A_0^{(1)} = \{0, 1\}$, $A_0^{(2)} = \{0, 1, 2\}$, $A_0^{(3)} = \{0, 1, 2\}$, ... $A_0^{(n)} = \{0, 1, 2\} = R_x$. For $i = 1 :$ $A_1^{(1)} = \{0, 2\}$, $A_1^{(2)} = \{0, 1, 2\}$, ... $A_1^{(n)} = \{0, 1, 2\} = R_x$. For $i = 2 : A_2^{(1)} = \{0\}$, $A_2^{(2)} = \{0, 1\}$, $A_2^{(3)} = \{0, 1, 2\}$, ... $A_2^{(n)} = \{0, 1, 2\} = R_x$. So, $m = 2, \forall n > m, \bigcup_{i \in R_x} A_i^{(n)} = R_x$.

(b) Write down the steady state equations.

$$\Pi_0 = \Pi_0(1 - a) + \Pi_1 b + \Pi_2,$$

$$\Pi_1 = \Pi_0 a$$

$$\Pi_2 = \Pi_1(1 - b),$$

$$\Pi_0 + \Pi_1 + \Pi_2 = 1.$$

(c) Solve the steady state equation.

$$\Pi_1 = \frac{a}{1 + 2a - ab}, \ \Pi_2 = \frac{a(1 - b)}{1 + 2a - ab}, \ \Pi_0 = \frac{1}{1 + 2a - ab}.$$

(d) Explain how you would use the Strong Law for Markov chains in this example. N is a random variable such $x_1, x_2, x_3, ...$ $\frac{1}{n}\sum_{i=1}^{n} x_i \to E(N)$ almost surely. $E(N) = \sum_j j\Pi_j$. Then, $x_i \in R_x$. $R_x = \{0, 1, 2\}$. The sequence of $x's$ is not independent and are not identically distributed.

Chapter 5

Operations Research II

Dr. Lawrence, College of William and Mary

Math 524, Spring 1992

Text used: Hillier, Frederick and Gerald J. Lieberman, *Introduction to Operations Research,* McGraw-Hill Publishing Company, 1990

5.1 Review of Probability Density Functions(PDF's)

- Uniform Distribution,

$$f(x) = \frac{1}{b-a}, a \leq x \leq b.$$

$$E(x) = \lambda = \frac{a+b}{2}$$

$$Var(x) = \frac{(b-a)^2}{12}.$$

- Exponential Distribution,

$$f(x) = \lambda e^{-\lambda x}, x > 0.$$

$$E(x) = \frac{1}{\lambda}$$

$$Var(x) = \frac{1}{\lambda^2}.$$

- Gamma Distribution,

$$f(x) = \frac{\lambda^n x^{n-1} e^{-\lambda x}}{n!}.$$

$$E(x) = \frac{n}{\lambda},$$

$$Var(x) = \frac{n}{\lambda^2}.$$

- Erlang Distribution,

$$f(x) = \lambda e^{-\sigma x} \frac{\lambda^n x^{n-1}}{(n-1)!}, x > 0.$$

- Poisson Distribution,

$$f(x) = \frac{\alpha x^n e^{-\alpha x}}{n!} \sim Poisson(\alpha x).$$

$$i.e. P(x(t) = 0) = e^{-\alpha t},$$

$$E(x(t)) = \alpha t.$$

5.2 Markov Chains

5.2.1 Stochastic Processes

A stochastic process is a family of random variables.

Example: $x_t; t \in I$ where each x_t is a random variable is a stochastic process. We will let I be 0,1,2,3,.... *Chain* is $x_0, x_1, x_2, ...$ Each x_i takes values in some finite set S, called the *state set.* Each x_i is a state. If A and B are events, $P(A|B)$ is the conditional probability of A given B. $P(A|B) = \frac{P(A \cap B)}{P(B)}$. The multiplier rule: $P(A \cap B) = P(A|B)P(B)$. The *Markov property:*

$$P(x_n = j | x_0 = i_0, x_1 = i_1, x_2 = i_2, ..., x_{n-1} = k) = P(x_n = j | x_{n-1} = k).$$

We will assume that our stochastic processes are Markov chains. If $\forall n, j, k, P(x_{n+1} = j | x_n = k) = P(x_1 = j | x_0 = k)$. The chain is said to be *stationary.* The mechanism does not change.

Example: Gambler's Ruin. A player plays a game in which he bets \$1.00 on each play if he has \$1.00 and does not have as much as \$5.00. On each play, there is a probability p that he will loss the \$1.00 that he bet and a probability q he will win \$1.00 and r that he will win \$2.00. Let p=0.7, q=0.2, and r=0.1. Let x_n be the person's wealth after the n-th play. The state space is {0,1,2,3,4,5}. $P_{ij} = P(x_1 = j | x_0 = i); i, j \in S$. The one step transition matrix

$$\text{IP} = [Pij] = \begin{array}{c|cccccc|} & 0 & 1 & 2 & 3 & 4 & 5 \\ \hline 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0.7 & 0 & 0.2 & 0.1 & 0 & 0 \\ 2 & 0 & 0.7 & 0 & 0.2 & 0.1 & 0 \\ 3 & 0 & 0 & 0.7 & 0 & 0.2 & 0.1 \\ 4 & 0 & 0 & 0 & 0.7 & 0 & 0.3 \\ 5 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}$$

Notice that all the rows total 1. Distribution of $x_0 : P(x_0 = i) = P_i, i \in 0, 1, 2, 3, 4, 5$. If the player starts with \$3.00, then$[P_0, ..., P_5] = [0, 0, 0, 1, 0, 0]$. Suppose there are 3 people waiting to play; 2 with \$4.00, one with \$2.00, and one with \$1.00. If the next player is chosen randomly, $[P_0, ..., P_5] = [0, \frac{1}{4}, \frac{1}{4}, 0, \frac{1}{2}, 0]$. 0 and 5 are called *absorbing states.* Let's look at states 0,1,2. P is the transition matrix $P = [P_{ij}]$. The initial distribution is $P = [P_0, P_1, P_2]$. $P(x_1 = 2) = P(x_1 = 2, x_0 = 0 \cup x_1 = 2, x_0 = 1 \cup x_1 = 2, x_0 = 2)$, $P(x_1 = 2) = P(x_1 = 2, x_0 = 0) + P(x_1 = 2, x_0 = 1) + P(x_1 = 2, x_0 = 2)$, $P(x_1 = 2) = P(x_0 = 0)P(x_1 = 2 | x_0 = 0) + P(x_0 = 1)P(x_1 = 2 | x_0 = 1) + P(x_0 = 2)P(x_1 = 2 | x_0 = 2) = P_0 P_{02} + P_1 P_{12} + P_2 P_{22}$.

$$[p_0, P_1, P_2] \begin{vmatrix} P_{00} & P_{01} & P_{02} \\ P_{10} & P_{11} & P_{12} \\ P_{20} & P_{21} & P_{22} \end{vmatrix}$$

5.2.2 Transition Matrices

Example: $\begin{vmatrix} 0.1 & 0 & 0 & 0.9 \\ 0.2 & 0.3 & 0.1 & 0.4 \\ 0 & 0 & 0 & 1 \\ 0.3 & 0.3 & 0.4 & 0 \end{vmatrix}$

$P(x_{n+1} = 3|x_n = 1) = 0.4$. Let x_0 have the distribution $P(x_0 = j) = P_j^0 = P_j$. $P(x_1 = i) = \sum_{i \in s} P_i P_{ij}$. $P^{(0)} = P = [P_1^{(0)}, P_2^{(0)}, ...]$. $P^{(0)}\mathrm{IP} = P^{(1)}$.

Example: $P_{ij}^{(2)} = P(x_2 = j|x_0 = i) = \sum_{k \in s} P_k^{(1)} P_{kj} = \sum_{k \in s} P_{ik} P_{kj} = \mathrm{IP}^2_{ij}$. The two step transition matrix $\mathrm{IP}^{(2)} = P_{ij}^{(2)} = \mathrm{IP}^2$. In general the n-step transition matrix is IP^n.

Example: Brand switching. there are three brands A, B, C, of a certain product on the market. If a person currently owns brand A, he is 4 times likely to buy brand A next as to switch brands. If he switches, he is equally likely to buy B or C. A person with B will switch to A with probability 0.3. A person with C will buy C again with probability 0.7 and switch to brand A with probability 0.3. Let the states be A=0, B=1, and C=2 and x_n be the brand owned after n steps.

$$\mathrm{IP} = \begin{vmatrix} 0.8 & 0.1 & 0.1 \\ 0.4 & 0.3 & 0.3 \\ 0.3 & 0 & 0.7 \end{vmatrix}$$

```
x  = probability A switches
4x = probability A does not switch
----------------------------------
5x = 1
```

Therefore, $x = \frac{1}{5}$. What is the probability that a person who owns brand A now will own brand B after the time after next?

$$\mathrm{IP}^2 = \begin{vmatrix} 0.71 & 0.11 & 0.18 \\ 0.53 & 0.13 & 0.34 \\ 0.45 & 0.03 & 0.52 \end{vmatrix}$$

Therefore, $P_{01}^{(2)} = 0.11$. What is the probability that a person owning brand B will own brand A next and then brand C? $P(x_1 = 0 \text{ and } x_2 = 2|x_0 = 1) = P(x_2 = 2|x_0 = 1, x_1 = 0)P(x_1 = 0|x_0 = 1) = P(x_2 = 2|x_1 = 0)P(x_1 = 0|x_0 = 1) = P_{02}P_{10} = (0.1)(0.4) = 0.04$. If a person with no experience chooses the first item at random, what is the probability that he will own brand A next? Brand C? $P = P^{(0)} = [\frac{1}{3}, \frac{1}{3}, \frac{1}{3}]$. What is $P_0^{(1)}$ and $P_2^{(1)}$?

$$p\mathrm{IP} = [\tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}] \begin{vmatrix} 0.8 & 0.1 & 0.1 \\ 0.4 & 0.3 & 0.3 \\ 0.3 & 0 & 0.7 \end{vmatrix}$$

$= [0.5, 0.133, 0.367]$. Therefore $P_0^{(1)} = 0.5$ and $P_2^{(1)} = 0.367$.

Example:

$$\begin{vmatrix} 0.3 & 0 & 0 & 0.5 & 0.2 \\ 0 & 0 & 0.6 & 0 & 0.4 \\ 0 & 0.8 & 0.2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0.5 & 0 & 0 & 0.5 \end{vmatrix}$$

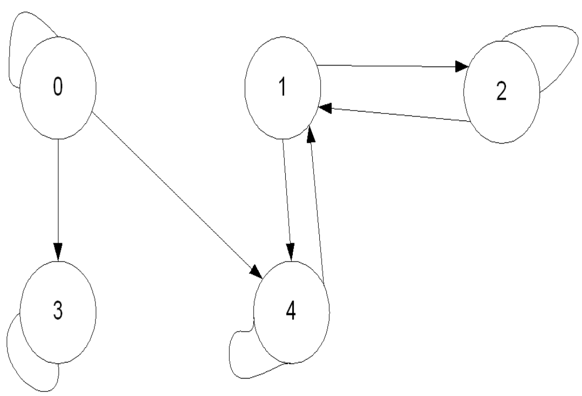


Figure 5.1: A state diagram.

See the state diagram in Figure 5.1.

5.2.3 Markov Terminology

Let 1,2,...,n be the states of a Markov chain. State i *leads* to j(or j is accessible from i) if it is possible to go from i to j. Conversely if any state leads to itself. If i leads to j and j leads to i then i and j *communicate.* If i communicates with j, then j communicates with i. If i communicates with j and j communicates with k then i communicates with k.

$$\begin{vmatrix} 0 & 0.1 & 0.3 & 0 & 0 & 0.6 \\ 0.2 & 0.3 & 0 & 0.5 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.6 & 0.4 & 0 \\ 0 & 0 & 0 & 0.2 & 0.2 & 0.6 \\ 0 & 0 & 0 & 0.3 & 0.5 & 0.2 \end{vmatrix}$$

See the state diagram in Figure 5.2. The communicating classes are: $\{1, 2\}$, $\{3\}$, $\{4, 5, 6\}$. A set of states T is *closed* if no state in T leads to a state outside T. e.g. $\{3\}$, $\{4,5,6\}$. A state i is *recurrent* if the probability of returning to state i given that it is in i is 1. A state that is not recurrent is called *transient.* If one state in a communicating class is recurrent, then they all are. If a chain has finitely many states, then the states in the communicating class are recurrent iff the class is closed. Therefore, states 1,2 are transient while states 3,4,5,6 are recurrent. If i and j are recurrent states which communicate, and the chain is in i then the state will go to j eventually with probability of 1. Suppose the chain is in state i with probability of 1 that it will eventually go to j. Let μ_{ij} be the expected number of steps needed to reach j. T_{ij} i number of states until chain reaches j if in state i. $\mu_{ij} = E(T_{ij})$. $\mu_{ij} = 1 + \sum_{k \neq j} P_{ik}\mu_{kj}, \forall i$.

Example: A factory has two machines of a certain type only one of which is used at a time. A machine in use on a day breaks down with a probability p. Let $q = 1 - p$. A broken machine requires 2 days to repair

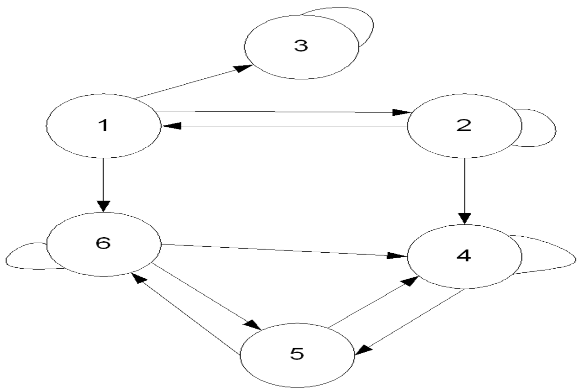


Figure 5.2: A state diagram.

not including the day on which it breaks down. Only one machine can be worked on at a time. The states are 0,1,2 number of machines broken down at the start of each day.

$$\begin{array}{c|ccc|} 0 & q & p & 0 \\ 1 & & & \\ 2 & & & \end{array}$$

$P(x_{n+1} = 0 | x_{n-2} = 0, x_{n-1} = 1, x_n = 1) = q$. $P(x_{n+1} = 0 | x_{n-1} = 0, x_n = 1) = 0$. Therefore, this is not a Markov chain. The states must be redefined. The second try at modeling follows. Let the states be, 0 = both working, 1 = one working and the other in first day of repair, 2 = one working and the other is second day of repair, and 3 = both down.

$$\mathrm{IP} = \begin{array}{c|cccc|} & 0 & 1 & 2 & 3 \\ \hline 0 & q & p & 0 & 0 \\ 1 & 0 & 0 & q & p \\ 2 & q & p & 0 & 0 \\ 3 & 0 & 1 & 0 & 0 \end{array}$$

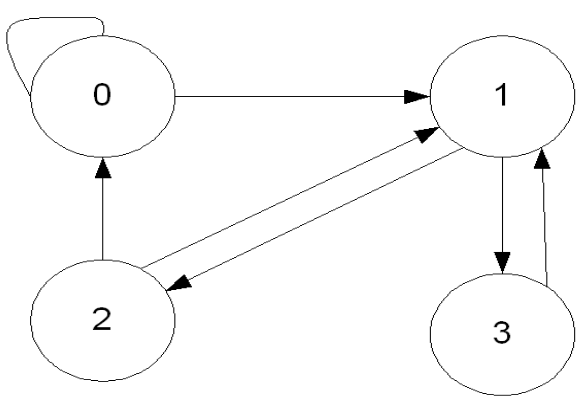


Figure 5.3: The second state diagram.

See Figure 5.3 for the second state diagram. Let T_{ij} be the number of steps needed to go from i to j. Let $E(T_{ij} = \mu_{ij})$. Then, $\mu_{ij} = 1 + \sum_{k \neq j} P_{ik} \mu_{kj}, \forall i$. Find μ_{03} in the above example. Let $p = 0.1$, and $q = 0.9$.

$\mu_{03} = 0.9\mu_{03} + 0.1\mu_{13} + 1$. $\mu_{13} = 0.9\mu_{23} + 1$. $\mu_{23} = 0.9\mu_{03} + 0.1\mu_{13} + 1$. $\mu_{33} = 1 + \mu_{13}$. Solve for μ_{03}. $0.01\mu_{03} = 1.1$. if $P_0 = [P(x_0 = 0), P(x_0 = 1), P(x_0 = 2), P(x_0 = 3)]$, then P_3(probability in the third step) $= [P(x_3 = 0), ..., P(x_3 = 3)]$. $P_3 = P_0\mathrm{IP}^3$. $\lim_{n\to\infty} P_{ij}^{(n)}$ = to what? A chain is irreductible if it has only one communicating class. That means that all states are recurrent. In most cases, an irreductible chain has a steady state distribution Π_i such that $\lim_{n\to\infty} P_{ij}^{(n)} \to \Pi_j$ and $\sum_j \Pi_j = 1$. $\Pi = \lim_{n\to\infty} P_n = \lim_{n\to\infty} P_0\mathrm{IP}^n$. $\Pi p = (\lim_{n\to\infty} P_0\mathrm{IP}^n)p = \lim_{n\to\infty} P_0\mathrm{IP}^{n+1} = \Pi$.

$$\lim_{n\to\infty} \mathrm{IP}^n = \begin{vmatrix} \Pi_0 & \Pi_1 & \Pi_3 & . & . & . & \Pi_n \\ \Pi_0 & \Pi_1 & \Pi_3 & . & . & . & \Pi_n \\ \Pi_0 & \Pi_1 & \Pi_3 & . & . & . & \Pi_n \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ \Pi_0 & \Pi_1 & \Pi_3 & . & . & . & \Pi_n \end{vmatrix}$$

Using the above example, the steady state solution is, $\Pi = \Pi\mathrm{IP}$, $\Pi = [\Pi_0, \Pi_1, \Pi_2, \Pi_3]$ $\Pi_0 = \overbrace{0.9\Pi_0 + 0.9\Pi_2}^{\text{Enter state on left}}$, $\Pi_1 = 0.1\Pi_0 + 0.1\Pi_2 + \Pi_3$, $\Pi_2 = 0.9\Pi_1$, $\Pi_3 = 0.1\Pi_1$, $\Pi_0 + \Pi_1 + \Pi_2 + \Pi_3 = 1$. Solve for $\Pi_0, ..., \Pi_3$. $\Pi_0 = 0.803, \Pi_1 = 0.099, \Pi_2 = 0.89, \Pi_3 = 0.10$. $\Pi_0 = \frac{1}{\mu_{00}}, \Pi_1 = \frac{1}{\mu_{11}}, \Pi_2 = \frac{1}{\mu_{22}}, \Pi_3 = \frac{1}{\mu_{33}}$.

5.2.4 Steady States

$\lim_{n\to\infty} P_{ij}^{(n)} = \Pi_j$; $\Pi = [\Pi_0, \Pi_1, \Pi_2, ..., \Pi_n]$.

$$\tilde{\Pi} = \begin{vmatrix} \Pi_0 & \Pi_1 & . & . & . & \Pi_n \\ \Pi_0 & \Pi_1 & . & . & . & \Pi_n \\ \Pi_0 & \Pi_1 & . & . & . & \Pi_n \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ \Pi_0 & \Pi_1 & . & . & . & \Pi_n \end{vmatrix}$$

$\lim_{n\to\infty} \mathrm{IP}^{(n)} = \tilde{\Pi}$. Use the brand switching example in the previous lecture.

$$\mathrm{IP} = \begin{vmatrix} 0.8 & 0.1 & 0.1 \\ 0.4 & 0.3 & 0.3 \\ 0.3 & 0 & 0.7 \end{vmatrix}$$

$\Pi = \Pi\mathrm{IP}$, $\Pi_0 + \Pi_1 + \Pi_2 + ... + \Pi_n = 1$. $\Pi_0 = 0.6176471, \Pi_1 = 0.0882353, \Pi_2 = 0.2941176$. $\mathrm{IP}^{(8)}$ is close to 4 places. $\mathrm{IP}^{(20)}$ is close to 7 places.

Example:

$$\mathrm{IP} = \begin{vmatrix} 0 & 0.3 & 0.7 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{vmatrix}$$

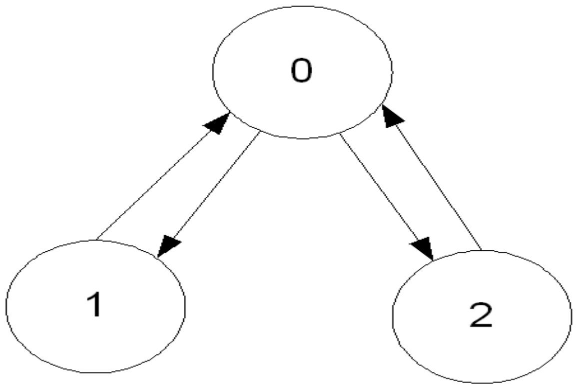


Figure 5.4: More state diagram examples.

See the state diagram in Figure 5.4.

$$P_{00} = \begin{cases} 1, & \text{if } n \text{ is even.} \\ 0, & \text{if } n \text{ is odd.} \end{cases}$$

$\lim_{n\to\infty} P_{00}^{(n)}$ diverges. For any recurrent state j, LCD$(n : P_{jj}^{(n)} > 0)$ is called the period of j. If j has a period of 1, it is called *aperiodic.* All the states in a communicating class have the same period. If a chain is irreductible and the states are aperiodic, then that is a steady-state distribution. If a chain is irreductible but not aperiodic, then there is no steady state solution but there is a unique *stationary solution.* That is, $\Pi = \Pi \mathrm{IP}$ and $\sum_j \Pi_j = 1$.

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=0}^{n} P_{ij}^{(n)} \to \Pi_j.$$

If for some n IP^n has all positive entries, then the states are aperiodic.

Example:

$$\begin{vmatrix} 0 & 0.1 & 0.9 & 0 \\ 0.8 & 0 & 0 & 0.2 \\ 0.3 & 0 & 0 & 0.7 \\ 0 & 0.6 & 0.4 & 0 \end{vmatrix}$$

See the state diagram in Figure 5.5. $n = \{$2,4,6,...,2n$\}$. Therefore it has a period of 2.

Example: See the state diagram in Figure 5.6. $n = \{$3,4,...$\}$. The LCD is 1. Therefore, the period is 1. Let x_n be an irreductible chain. Let $C(j)$ be the cost of having the chain in state j at any step.

$$E\left(\frac{1}{N}\sum_{n=1}^{N} C(x_n)\right).$$

$$\lim_{N\to\infty} E\left(\frac{1}{N}\sum_{n=1}^{N} C(x_n)\right) = \lim_{N\to\infty} \sum_{k=0}^{m} \frac{1}{N} \sum_{n=1}^{N} C(k)P(x_n = k).$$

y is a random variable that takes on values $\{q_1, q_2, ..., q_t\}$. Let h(y) be a real valued function. Z = h(y). Say

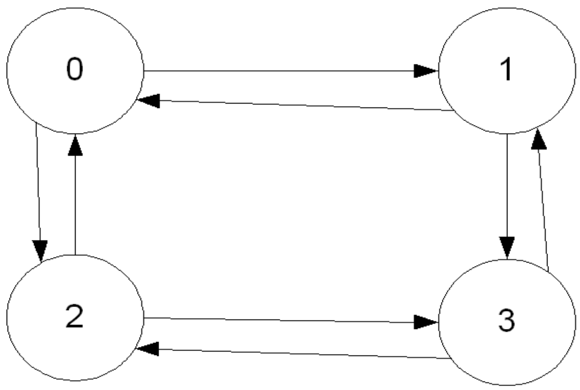


Figure 5.5: More state diagram examples.

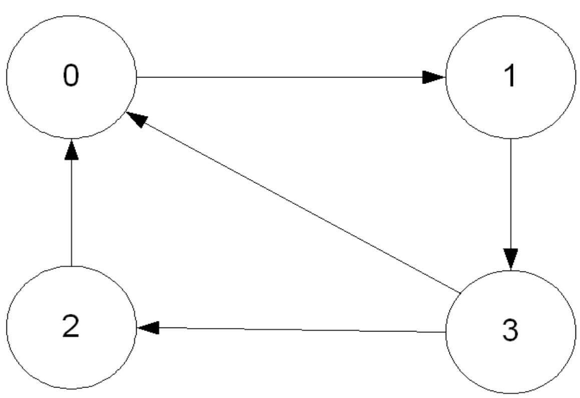


Figure 5.6: More state diagram examples.

y has a distribution of $f(q_i) = P(y = q_i) = \alpha_i$.

$$E(Z) = E(h(y)) = \sum_{j=0}^{t} h(q_j)P(y = q_j) = \sum_{j=0}^{t} h(q_j)f(q_j) = \sum_{j=1}^{t} H(q_j)\alpha_j.$$

$$\lim_{N\to\infty} \sum_{k=0}^{m} \frac{1}{N} \sum_{n=1}^{N} C(k) \sum_{j=0}^{m} p_j^{(0)} p_{jk}^{(n)} = \sum_{j=0}^{m} P_j^{(0)} \sum_{k=0}^{m} C(k) \left(\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} p_{jk}^{(n)} \right) \to \Pi_k.$$

5.2.5 Expected Costs

Suppose we have x_n, $C(j), j \in S = 0, 1, l ... m$.

$$\lim_{N\to\infty} E\left(\frac{1}{N}\sum_{n=1}^{N} C(x_n)\right) = ... = \sum_{k=0}^{n} C(k) \sum_{j=0}^{n} P_j^{(0)} \Pi_k = \sum_{k=0}^{n} C(k)\Pi_k \sum_{j=0}^{n} P_j^{(0)} = \sum_{k=0}^{n} C(k)\Pi_k.$$

Let's use an earlier example.

$$\mathrm{IP} = \begin{vmatrix} 0.9 & 0.1 & 0 & 0 \\ 0 & 0 & 0.9 & 0.1 \\ 0.9 & 0.1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{vmatrix}$$

We get, $\Pi_0 = 0.802$, $\Pi_1 = 0.099$, $\Pi_2 = 0.089$, $\Pi_3 = 0.01$. Suppose that C(0) = 0, C(1) = 3, C(2) = 5, and C(3) = 35. The expected daily average cost in the long run is

$$\sum_{k=0}^{n} C(k)\Pi_k = 3(0.099) + 5(0.089) + 35(0.01) = 1.089.$$

The cost could be random also. e.g. C(k,D). The long run expected cost per step is

$$\sum_{k=0}^{n} E(C(k, D))\Pi_k.$$

Using the same example, let the demand for the product for which the machines are used to be D. Assume D is uniform on 50 to 150. Let C(0,0)=0,

$$C(1, D) \begin{cases} 4(D - 75), & \text{if } D \geq 75 \\ 0, & \text{if } D < 75 \end{cases} \tag{5.1}$$

$$C(2, D) \begin{cases} 2(D - 25), & \text{if } D \geq 125 \\ 0, & \text{if } D < 125 \end{cases} \tag{5.2}$$

$$C(3, D) = 10D.$$

K(1) is the expected cost of being in state 1 for one day. $f_0(s)$ is the pdf.

$$k(1) = E(C(1, D)) = \int_{-\infty}^{\infty} C(1, s)f_0(s)ds = \int_{75}^{150} \frac{4(s - 75)}{100} ds = \frac{1}{25}\left[\frac{s^2}{2} - 75s\right]_{75}^{150} = 0 - \frac{75}{25}\left(\frac{75}{2} - 75\right) = 112.5.$$

$$k(2) = E(C(2, D)) = \int_{-\infty}^{\infty} C(2, s)f_0(s)ds = \int_{25}^{150} \frac{2(s - 25)}{100} ds = ... = 6.25.$$

$$k(3) = E(C(3, D)) = \int_{-\infty}^{\infty} C(3, s) f_0(s) ds = 10(100) = 1000.$$

The long run expected cost is = (0.099)(112.5) + (0.089)(6.25) + (0.01)(1000). Let x_n be a Markov chain with transient states 0,1,2...,k, an absorbing state r and the other states being recurrent. What is the probability of eventually being in state r? Absorbing probabilities: Let $f_{ir} = P(x_n = r \text{ for some } n | x_0 = i)$.

$$f_{ir} = P_{ir} + \sum_{j=0}^{k} P_{ij} f_{jr}, i = 0, ..., k.$$

Let m be recurrent. $m = \Pi_r = P_{im} = 0$. Suppose,

$$\mathrm{IP} = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0.2 & 0.3 & 0.1 & 0.4 \\ 0 & 0 & 1 & 0 \\ 0.1 & 0.6 & 0 & 0.3 \end{vmatrix}$$

There are two absorbing states, and two transient states.

$$f_{10} = 0.2 + (0.3 f_{10} + 0.4 f_{30}),$$

$$f_{30} = 0.1 + (0.6 f_{10} + 0.3 f_{30}).$$

Solving the system of equations simultaneously yields,

$$F_{30} = \frac{1}{2},$$

and

$$f_{10} = \frac{4}{7}.$$

5.2.6 Absorbing States

Example: Consider the state diagram in Figure 5.7. What is the probability of being in state 4? Let X_x be a Markov chain with states 1,2,3,4,...,m. Let state m be the absorbing state and let states $i_1, ..., i_k$ be transient states. Let f_{jk} be the probability that the chain reaches state k at some point given that it starts in state j. Use first step analysis.

$$f_{i,m} = P_{i,m} + \sum_{j=1}^{k} P_{i,j} f_{i,m}.$$

The above equation is the form for each transient state. Note that the probability of being in m from any recurring states is 0. See Figure 5.8 for the state diagram used in the example.

	1	2	3	4	5
0	1	0	0	0	0
1	0.1	0.3	0.2	0	0.4
2	0.3	0.2	0	0.4	0.1
3	0.5	0	0.1	0	0.4
4	0	0	0	0	1

What is the probability of reaching state 4? $f_{14} = 0.4 + 0.3 f_{14} + 0.2 f_{24}$, $f_{24} = 0.1 + 0.2 f_{14} + 0.4 f_{34}$, $f_{34} = 0.4 + 0.1 f_{24} + 0.2 f_{14}$.

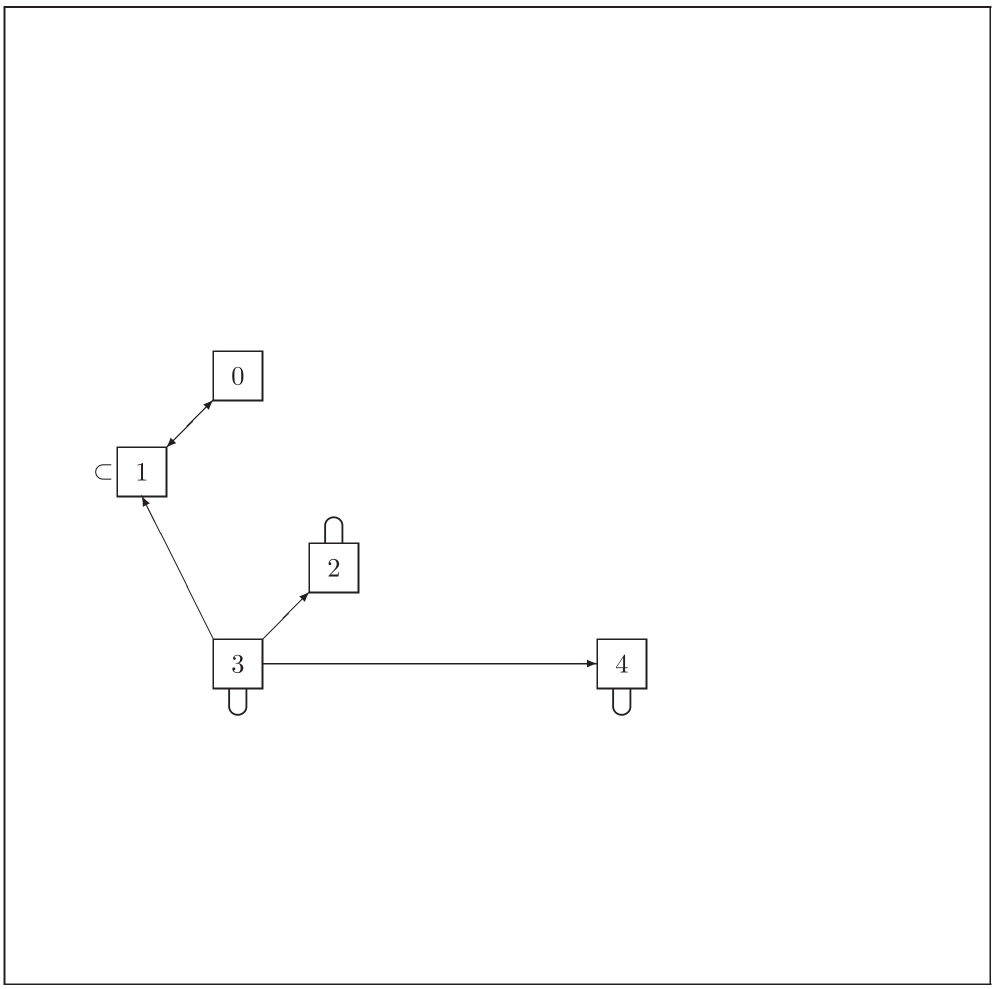


Figure 5.7: Absorbing States

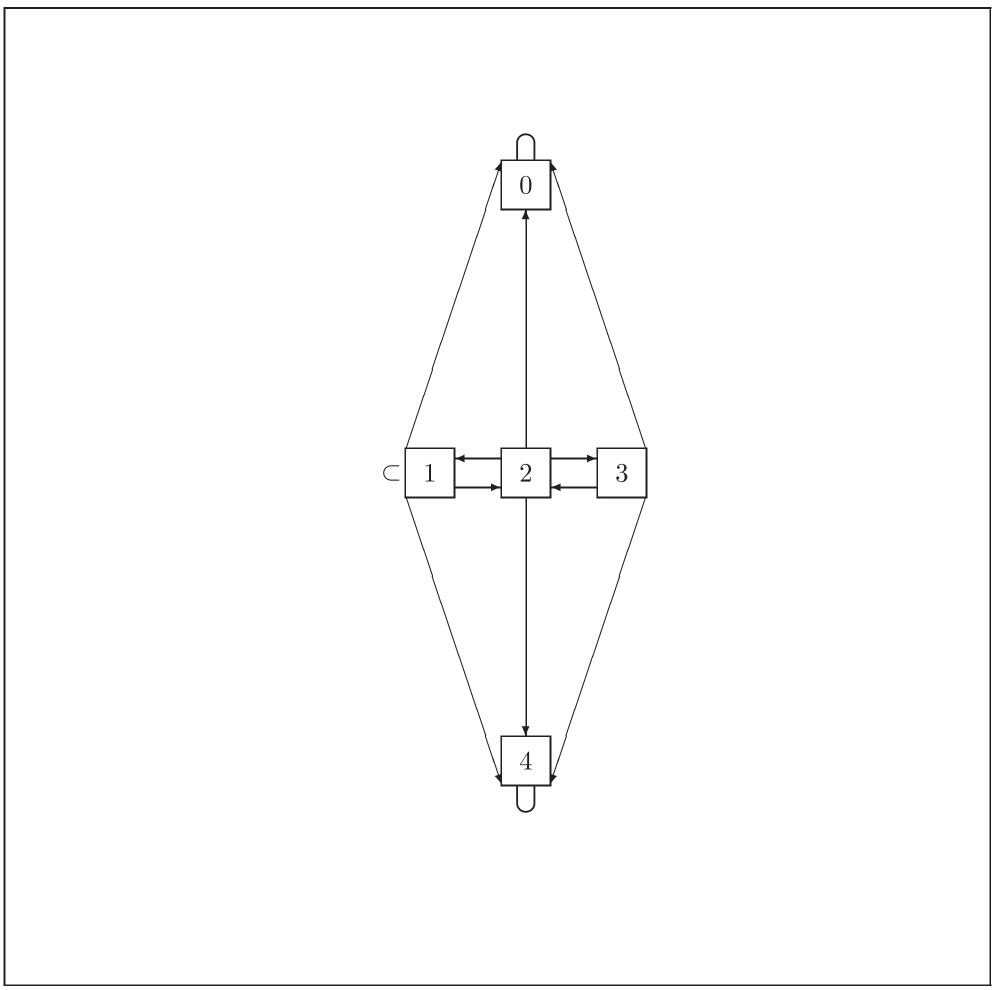


Figure 5.8: A State Diagram

Example: Three Russian men fight a three way dual. On each shot each survivor shoots at the best shot among the other survivors. The shots are independent and the hit probabilities are $A = \frac{1}{2}, B = \frac{1}{3}, C = \frac{1}{6}$. Model this situation. The states are A,B,C all are alive = 1. AC = 2. BC = 3. A = 4, B= 5, C = 6, = 7. Note that there is no AB. $(1,1) = \frac{1}{2}\frac{2}{3}\frac{5}{6} = \frac{5}{18}$. $(1,2) = \frac{1}{2}\frac{2}{3}\frac{5}{6} = \frac{5}{18}$. $(1,6) = \frac{1}{2}\frac{1}{3}\frac{5}{6} + \frac{1}{2}\frac{2}{3}\frac{1}{6} + \frac{1}{2}\frac{1}{3}\frac{1}{6} = \frac{2}{9}$.

	1	2	3	4	5	6	7
1	$\frac{5}{18}$	$\frac{5}{18}$	$\frac{2}{9}$	0	0	$\frac{2}{9}$	0
2	0	$\frac{5}{12}$	0	$\frac{5}{12}$	0	$\frac{1}{12}$	$\frac{1}{12}$
3	0	0	$\frac{5}{9}$	0	$\frac{5}{18}$	$\frac{1}{9}$	$\frac{1}{18}$
4	0	0	0	1	0	0	0
5	0	0	0	0	1	0	0
6	0	0	0	0	0	1	0
7	0	0	0	0	0	0	1

Find the probability that C is the lone survivor. The question is asking for f_{16}. $f_{16} = \frac{2}{9} + \frac{5}{18} f_{16} + \frac{5}{18} f_{26} + \frac{2}{9} f_{36}$, $f_{26} = \frac{1}{12} + \frac{5}{12} f_{26}$, $f_{36} = \frac{1}{9} + \frac{5}{9} f_{56}$. See Figure 5.9.

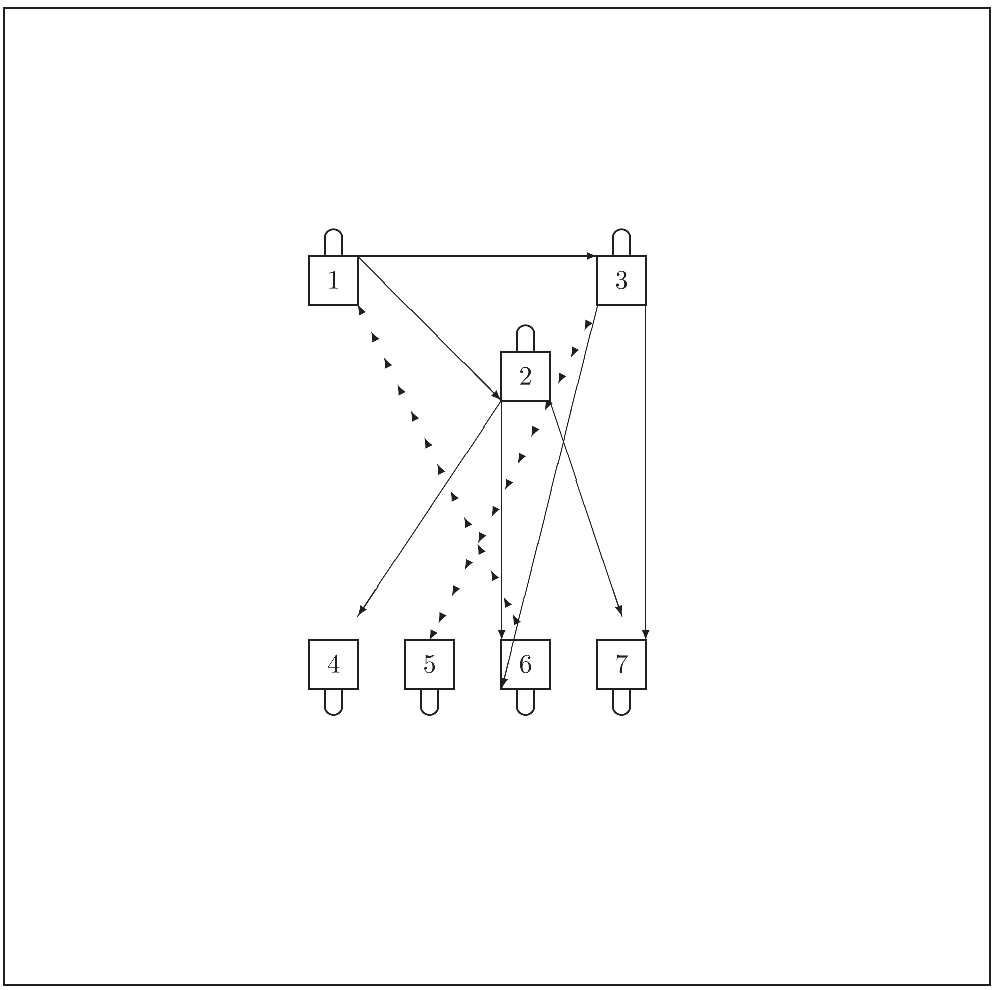


Figure 5.9: A State Diagram

absorbing state	A4	B5	C6	7
probability	0.2747	0.1923	0.4396	0.0934

5.2.7 Homework and Answers

Problems 2, 3, 6, 7, 9, 11, 14, 15, 18, 21, 23, 24.

1. A weather service in a certain area classifies each winter day as rainy(R), snowy(S), or clear(C) and models the daily weather as a Markov chain with states R, S, and C and transition matrix

$$\begin{array}{ccc} R & S & C \\ \end{array}$$
$$\begin{vmatrix} 0.30 & 0.15 & 0.55 \\ 0.15 & 0.15 & 0.70 \\ 0.05 & 0.05 & 0.90 \end{vmatrix}$$

   (a) If today is clear, find the expected number of days until the next rainy day.

   (b) If today is clear, find the expected number of clear days until the next day that is not clear. Hint: for $|a| < 1, \sum_{n=1}^{\infty} na^{n-1} = \frac{1}{(1-a)^2}$.

   (c) In the long run what fraction of the time is the weather clear?

   (a)

$$\mu_{SR} = 1 + 0.15\mu_{SR} + 0.70\mu_{CR},$$

$$\mu_{CR} = 1 + 0.05\mu_{SR} + 0.9\mu_{CR}.$$

   Using algebra and substitution,

$$0.85\mu_{SR} - 0.70\mu_{CR} = 1,$$

$$-0.5\mu_{SR} + 0.1\mu_{CR} = 1.$$

$$\mu_{SR} = 16.$$

$$\mu_{CR} = 18.$$

   Expected time until rain is 18 days.

   (b) Let k be the number of clear days after today until the next rainy day or snowy day.

$$f_k(n) = P(k = n) = P(X_1 = C, X_2 = C, ..., X_n = C, X_{n+1} \neq C | X_0 = ?) = p_{CC}^n(1 - p_{CC}) =$$

$$0.9^n(0.1), \text{for } n = 0, 1, 2, 3, ...$$

   So,

$$E(k) = \sum_{n=0}^{\infty} n(0.9^n)(0.1) = (0.9)(0.1)\sum_{n=0}^{\infty} n(0.9^{n-1}) = (0.9)(0.1)\frac{1}{(1-0.9)^2} = \frac{0.9}{0.1} = 9.$$

   See hint.

(c) $\Pi = \Pi P$ yields:

$$\Pi_R = 0.3\Pi_R + 0.15\Pi_S + 0.05\Pi_C,$$

$$\Pi_S = 0.15\Pi_R + 0.15\Pi_S + 0.05\Pi_C,$$

$$\Pi_C = 0.55\Pi_R + 0.70\Pi_S + 0.90\Pi_C.$$

These with $\Pi_R + \Pi_S + \Pi_C = 1$ gives

$$\Pi_R = 0.075,$$

$$\Pi_S = 0.064,$$

$$\Pi_C = 0.861.$$

In the long run, the weather is clear 0.861 of the days.

2. A small firm extends credit at the beginning of each month to customers who pay off the debt in a single payment at the end of the month. This happens with probability 0.70. Otherwise the account is classified as 1 month old debt. At the beginning of a month, one month old debt is paid with probability 0.50 or it becomes a two month old debt. Two month old debts become three month old debts with a probability of 0.80. Three month old debts are paid with a probability of 0.60. Otherwise, it is written off as a bad debt.

   (a) Model this as a Markov chain giving the meaning of the states and the transition matrix.

   (b) Find the probability that a new debt will eventually become a bad debt.

   (a) States: 0 = new, 1 = one month old, 2 = two months old, 3 = three months old, 4 = paid, 5 = bad debt.

$$\begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{array}\left|\begin{array}{cccccc} 0 & 0.3 & 0 & 0 & 0.7 & 0 \\ 0 & 0 & 0.5 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0.8 & 0.2 & 0 \\ 0 & 0 & 0 & 0 & 0.6 & 0.4 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right|$$

   (b)

$$f_{05} = 0.3f_{15},$$

$$f_{15} = 0.5f_{25},$$

$$f_{25} = 0.8f_{35},$$

$$f_{35} = 0.4.$$

Using substitution, the following values are obtained.

$$f_{35} = 0.4,$$

$$f_{25} = 0.32,$$

$$f_{15} = 0.16,$$

$$f_{05} = .048,$$

F_{05} is the probability that a new debt will turn bad.

Problem 2: Assume the probability of rain tomorrow is α if it is raining today,and assume that the probability of its being clear tomorrow is β if it is clear today.

1. Determine the one-step transition matrix of the Markov chain.
2. Find the two-step transition matrix.
3. Find the steady-state probabilities.

1.
$$P = \begin{vmatrix} \alpha & 1-\alpha \\ 1-\beta & \beta \end{vmatrix}$$

2.
$$P^2 = \begin{vmatrix} \alpha^2 + (1-\alpha)(1-\beta) & \alpha(1-\alpha)+\beta(1-\alpha) \\ \alpha(1-\beta)+\beta(1-\beta) & (1-\alpha)(1-\beta)+\beta^2 \end{vmatrix} = \begin{vmatrix} \alpha^2 + (1-\alpha)(1-\beta) & (\alpha+\beta)(1-\alpha) \\ (\alpha+\beta)(1-\beta) & \beta^2+(1-\alpha)(1-\beta) \end{vmatrix}$$

3.
$$\Pi_0 = \alpha\Pi_0 + (1-\beta)\Pi_1,$$
$$\Pi_1 = (1-\alpha)\Pi_0 + \beta\Pi_1.$$

From the above two equations we get,

$$(1-\alpha)\Pi_0 - (1-\beta)\Pi_1 = 0,$$
$$\Pi_0 + \Pi_1 = 1,$$
$$\Pi_1 = 1 - \Pi_0.$$

Substituting Π_1, we get,

$$(1-\alpha)\Pi_0 - (1-\beta)(1-\Pi_0) = 0,$$
$$[(1-\alpha)+(1-\beta)]\Pi_0 = 1-\beta,$$
$$\Pi_0 = \frac{1-\beta}{2-\alpha-\beta}.$$
$$\Pi_1 = \frac{1-\alpha}{2-\alpha-\beta}.$$

Problem 3: Consider the stock market model presented in Sec. 15.3. Whether or not the stock goes up tomorrow depends upon whether or not it increased today *and* yesterday. If the stock has increased for the past two days, it will increase tomorrow with probability α_1. If the stock increased today but decreased yesterday, it will increase tomorrow with probability α_2. If the stock decreased today but increased yesterday, it will increase tomorrow with probability α_3. Finally, if the stock decreased for the past two days, it will increase tomorrow with probability α_4.

1. Determine the one-step transition matrix of the Markov chain.
2. Find the steady-state probabilities.

1. States: 0 = increase yesterday and today 1 = decrease yesterday and increase today 2 = increase yesterday and decrease today 3 = decrease yesterday and today

$$\begin{vmatrix} 0 & 1 & 2 & 3 \\ \alpha_1 & 0 & 1-\alpha_1 & 0 \\ \alpha_2 & 0 & 1-\alpha_2 & 0 \\ 0 & \alpha_3 & 0 & 1-\alpha_3 \\ 0 & \alpha_4 & 0 & 1-\alpha_4 \end{vmatrix}$$

2.

$$\Pi_0 = \alpha_1\Pi_0 + \alpha_2\Pi_1$$

$$\Pi_1 = \alpha_3\Pi_2 + \alpha_4\Pi_3$$

$$\Pi_2 = (1-\alpha_1)\Pi_0 + (1-\alpha_2)\Pi_1$$

$$\Pi_3 = (1-\alpha_3)\Pi_2 + (1-\alpha_4)\Pi_3$$

$$\Pi_0 + \Pi_1 + \Pi_2 + \Pi_3 = 1$$

Using algebra, the following equations are obtained:

$$\Pi_1 = \frac{1-\alpha_1}{\alpha_2}\Pi_0,$$

$$\Pi_2 = \left[(1-\alpha_1) + (1-\alpha_2)\frac{1-\alpha_1}{\alpha_2}\right]\Pi_0 = \frac{1-\alpha_0}{\alpha_2}\Pi_0(1-\alpha_1)$$

$$\Pi_3 = \frac{1-\alpha_3}{\alpha_4}\Pi_2 = \left[\frac{(1-\alpha_1)(1-\alpha_3)}{\alpha_2\alpha_4}\right]\Pi_0$$

$$1 = \left[1 + \frac{1-\alpha_1}{\alpha_2} + \frac{1-\alpha_1}{\alpha_2} + \frac{(1-\alpha_1)(1-\alpha_3}{\alpha_2\alpha_4}\right]\Pi_0 = \frac{\alpha_2\alpha_4 + 2\alpha_4(1-\alpha_1) + (1-\alpha_3)}{\alpha_2\alpha_4}$$

$$\Pi = \frac{1}{\alpha_2\alpha_4 + 2\alpha_4(1-\alpha_1) + (1-\alpha_1)(1-\alpha_3)} \times [\alpha_2\alpha_4, \alpha_4(1-\alpha_1), \alpha_4(1-\alpha_1), (1-\alpha_1)(1-\alpha_3)]$$

Problem 6: Determine the classes of the Markov chains and whether or not they are recurrent.

$$\mathbf{A} = \begin{vmatrix} 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \end{vmatrix}$$

$$\mathbf{B} = \begin{vmatrix} 0 & 0 & 1 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 1 & 0 \end{vmatrix}$$

See the state diagrams in Figure 5.10 and Figure 5.11.
Only one class {0,1,2,3} which must be recurrent.
Only one class {0,1,2} which must be recurrent.

Problem 7: Determine the classes of the Markov chain and whether or not they are recurrent in Figure 5.12 and in Figure 5.13.

$$\begin{vmatrix} \frac{1}{4} & \frac{3}{4} & 0 & 0 & 0 \\ \frac{3}{4} & \frac{1}{4} & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & \frac{3}{4} & \frac{1}{4} \\ 0 & 0 & 0 & \frac{1}{4} & \frac{3}{4} \end{vmatrix}$$

Class {0,1} is recurrent since it is closed. Class {2} is transient since it is not closed. Class {3,4} is recurrent since it is closed.

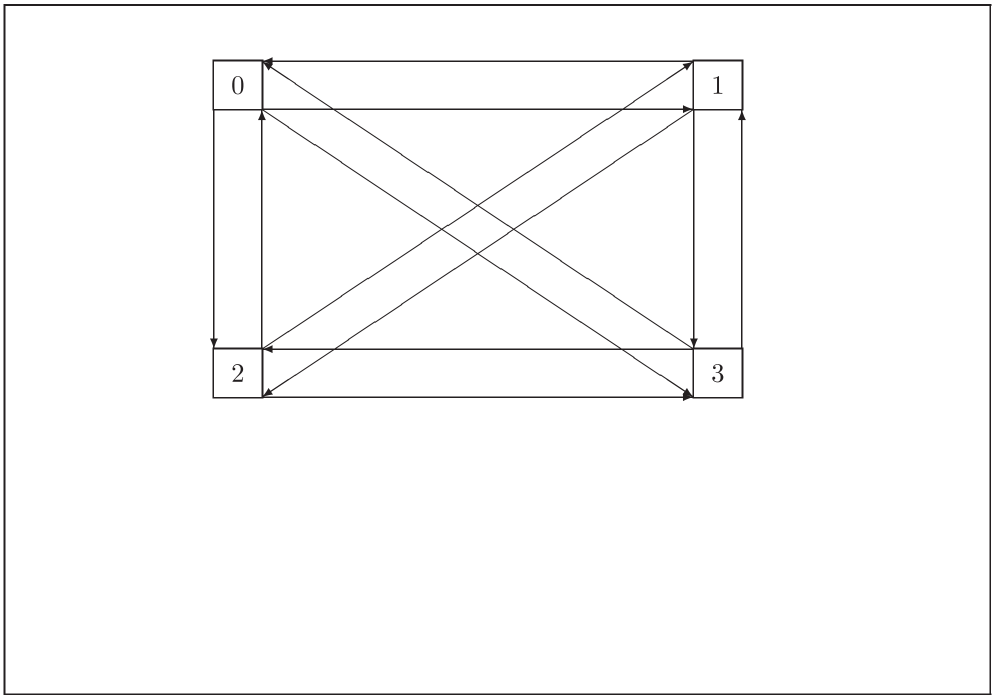


Figure 5.10: Recurrence

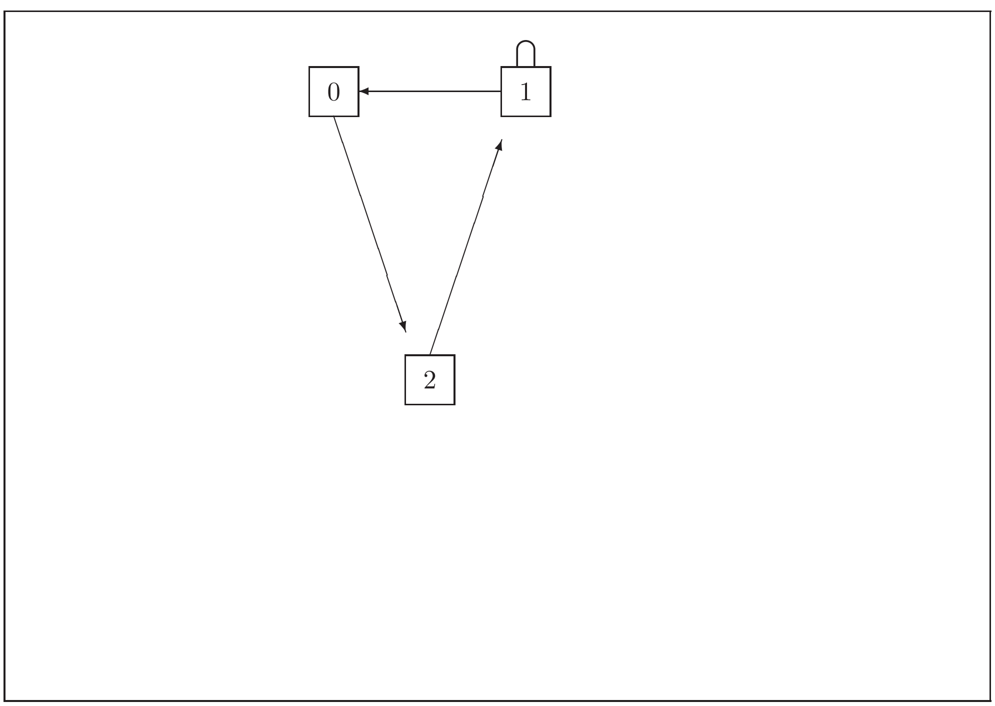


Figure 5.11: Recurrence

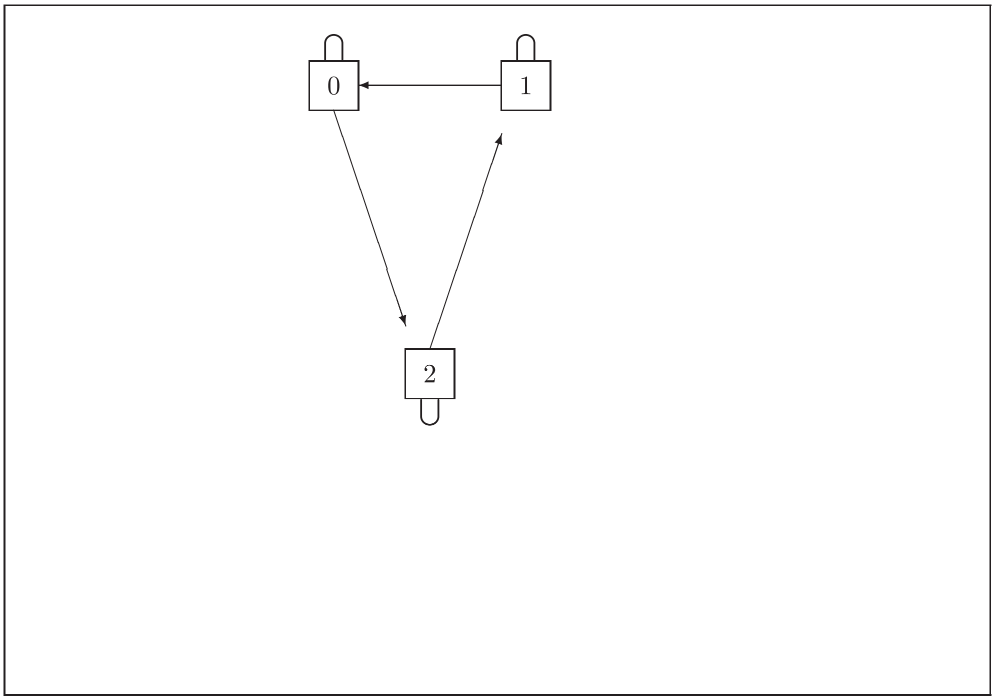


Figure 5.12:

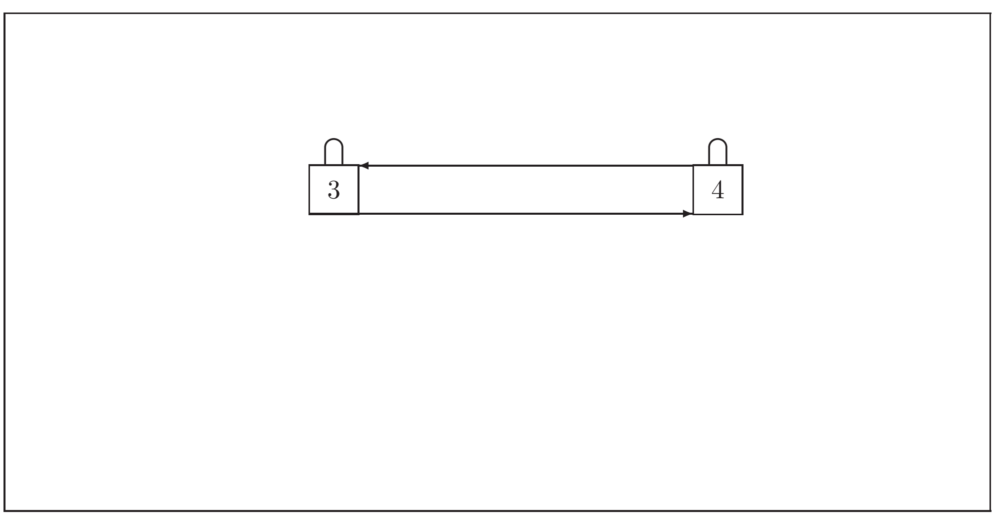


Figure 5.13:

Problem 9: A transition matrix **P** is said to be doubly stochastic if the sum over each column equals 1; that is,

$$\sum_{i=0}^{M} p_{ij} = 1, \forall j.$$

If such a chain is irreductible, aperiodic, and consists of $M+1$ states, show that

$$\pi_j = \frac{1}{M+1}, \text{ for } j = 0, 1, ..., M.$$

Let $\Pi_j = \alpha$ for $j = 0, 1, ..., n$. We note that $\Pi = \Pi\rho$ gives

$$\sum_{i=0}^{M} \Pi_i \rho_{ij} = \sum_{i=0}^{M} \alpha\rho_{ij} = \alpha \sum_{i=0}^{M} \rho_{ij} = \alpha = \Pi_j.$$

So the system $\Pi = \Pi\rho$ is satisfiable. Thus,

$$1 = \sum_{j=0}^{M} \Pi_j = (M+1)\alpha$$

so $\alpha = \frac{1}{M+1}, \Pi_j = \frac{1}{M+1}$ for all j.

Consider the problem of searching a linked list. Analysis of a doubly stochastic matrix shows that searching a circular doubly linked list has no statistical advantages over a non-circular doubly linked list using the proof in problem 9.

Problem 11: The leading brewery on the West Coast(labeled A) has hired an operations research analyst to analyze its market position. It is particularly concerned about its major competitor(labeled B). The analyst believed that brand switching can be modeled as a Markov chain using three states, with states A and B representing customers drinking beer produced from the aforementioned breweries and state C representing all other brands. Data are taken monthly, and the analyst has constructed the following transition matrix from past data.

$$\begin{vmatrix} A & B & C \\ 0.70 & 0.20 & 0.10 \\ 0.20 & 0.75 & 0.05 \\ 0.10 & 0.10 & 0.80 \end{vmatrix}$$

What are the steady-state market shares for the two major breweries?

$$\Pi_A = 0.7\Pi_A + 0.2\Pi_B + 0.1\Pi_C,$$

$$\Pi_B = 0.2\Pi_A + 0.75\Pi_B + 0.1\Pi_C,$$

$$\Pi_C = 0.1\Pi_A + 0.05\Pi_B + 0.8\Pi_C,$$

$$\Pi_A + \Pi_B + \Pi_C = 1.$$

$$\Pi_A = 0.3462.$$

$$\Pi_B = 0.3846.$$

$$\Pi_C = 0.2692.$$

Problem 14: A computer is inspected at the end of every hour. It is found to be either working(up) or failed(down). If the computer is found to be up, the probability of it remaining up for the next hour is 0.90. If it is down, repair action, which may require more than an hour, is taken. Whenever the machine is down(regardless of how long it has been down), the probability of it still being down an hour later is 0.35.

1. Show that this is a Markov chain and find the transition matrix.
2. Find the steady-state probabilities of the machine being up and down.

0: up, 1: down.

1. $\begin{vmatrix} 0.90 & 0.10 \\ 0.65 & 0.35 \end{vmatrix}$

2.

$$\Pi_0 = 0.90\Pi_0 + 0.65\Pi_1,$$

$$\Pi_1 = 0.10\Pi_0 + 0.35\Pi_1,$$

$$\Pi_0 + \Pi_1 = 1.$$

$$\Pi_0 = 0.8667.$$

$$\Pi_1 = 0.1333.$$

Problem 15: Consider the following blood inventory problem facing a hospital. Suppose there is need for a rare blood type,e.g. type AB, Rh negative blood. Suppose the demand over a three-day period is given by $P(D = 0) = 0.40$, $P(D = 1) = 0.30$, $P(D = 2) = 0.20$, and $P(D = 3) = 0.10$.

Note that the expected demand is then 1 unit. Suppose that there are three days between deliveries. The hospital proposes a policy of receiving one pint at each delivery and uses the oldest blood first, i.e. it uses a FIFO policy (first in, first out). If more blood is required than is on hand, an expensive emergency delivery is made. Blood is discarded if it is still on the shelf after 21 days. Denote the state of the system as the number of pints on hand just after a delivery. Noting that the largest state is 7:

1. Find the transition matrix.
2. Find the steady-state probabilities.

1. States {1,2,3,4,5,6,7}

$$P = \left|\begin{array}{ccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ \hline 0.6 & 0.4 & 0 & 0 & 0 & 0 & 0 \\ 0.3 & 0.3 & 0.4 & 0 & 0 & 0 & 0 \\ 0.1 & 0.2 & 0.3 & 0.4 & 0 & 0 & 0 \\ 0 & 0.1 & 0.2 & 0.3 & 0.4 & 0 & 0 \\ 0 & 0 & 0.1 & 0.2 & 0.3 & 0.4 & 0 \\ 0 & 0 & 0 & 0 & 0.1 & 0.2 & 0.7 \end{array}\right|$$

2. $\Pi = \Pi P$ and $\sum_{j=1}^{7} \Pi_j = 1$ yields $\Pi_1 = 0.1389, \Pi_2 = 0.1389, \Pi_3 = 0.1390, \Pi_4 = 0.1383, \Pi_5 = 0.1411, \Pi_6 = 0.132, \Pi_7 = 0.1736$.

Problem 18: A production process contains a machine that deteriorates rapidly in both quality and output under heavy usage, so that it is inspected at the end of each day. Immediately after inspection, the condition of the machine is noted and classified into one of four possible states:

State	Condition
0	Good as new
1	Operable - minimum deterioration
2	Operable - major deterioration
3	Inoperable and replaced by a good-as-new machine

The process can be modeled as a Markov chain with transition matrix given by

State	0	1	2	3
0	0	$\frac{7}{8}$	$\frac{1}{16}$	$\frac{1}{16}$
1	0	$\frac{3}{4}$	$\frac{1}{8}$	$\frac{1}{8}$
2	0	0	$\frac{1}{2}$	$\frac{1}{2}$
3	1	0	0	0

1. Find the steady-state probabilities.
2. If the costs of being in states 0,1,2,3 are \$0, \$1,000, \$3,000, and \$6,000, respectively, what is the long-run expected average cost per day?

1.

$$\begin{aligned}
&\Pi_0 = \Pi_3,\\
&\Pi_1 = \frac{7}{8}\Pi_0 + \frac{3}{4}\Pi_1,\\
&\Pi_2 = \frac{1}{16}\Pi_0 + \frac{1}{8}\Pi_1 + \frac{1}{2}\Pi_2,\\
&\Pi_3 = \frac{1}{16}\Pi_0 + \frac{1}{8}\Pi_1 + \frac{1}{2}\Pi_2,\\
&\Pi_0 + \Pi_1 + \Pi_2 + \Pi_3 = 1.
\end{aligned}$$

Solution:

$$\Pi_0 = 0.1538, \Pi_1 = 0.5385, \Pi_2 = 0.1538, \Pi_3 = 0.1538.$$

2.

$$(1,000)(0.5385) + (3,000)(0.1538) + (6,000)(0.1538) = 1923.08.$$

Problem 21: Consider the following (k, Q) inventory policy. Let D_1, $D_2, \ldots$, be the demand for a product in periods 1,2,..., respectively. If the demand during a period exceeds the number of items available, this unsatisfied demand is bocklogged; i.e. it is filled when the next order is received. Let $Z_n (n = 0, 1, \ldots)$ denote the amount of inventory on hand minus the number of units bocklogged before ordering at the end of period $n (Z_0 = 0)$. If Z_n is zero or positive, no orders are bocklogged. If Z_n is negative, then $-Z_n$ represents the number of bocklogged units and no inventory is on hand. If at the end of period n, $Z_n < k = 1$, an order is placed for $2m (Qm$ in general) units, where m is the smallest integer such that $Z_n + 2m \geq 1$.(The amount ordered is the smallest integral multiple of 2, which brings the level to at least 1 unit). Let D_n be independent and identically distributed random variables taking on the values, 0,1,2,3,4, each, with probability $\frac{1}{5}$. Let X_n denote the amount of stock on hand *after* ordering at the end of period $n (X_0 = 2)$. It is evident that

$$X_n \begin{cases} X_{n-1} - D_n + 2m, & \text{if } X_{n-1} - D_n < 1 \\ X_{n-1} - D_n, & \text{if } X_{n-1} - D_n \geq 1 \end{cases} \tag{5.3}$$

for $n = 1, 2, 3, ...,$ and X_n(n=0,1,...) is a Markov chain with only two states: 1 and 2. [The only time that ordering will take place is when $Z_n = 0, -1, -2, -3$, in which case 2,2,4, and 4 units are ordered, respectively, leaving $X_n = 2, 1, 2, 1$, respectively. In general, for any (k, Q) policy, the possible states are $k, k+1, k+3, ..., k+Q-1$.]

1. Find the one-step transition matrix.

2. Find the stationary probabilities(see Prob. 9).

3. Suppose that the ordering cost is given by $(2+2m)$ if an order is placed and zero otherwise. The holding cost per period is Z_n if $Z_n \geq 0$, and zero otherwise. The shortage cost per period is $-4Z_n$ if $Z_n < 0$ and zero otherwise. Find the (long-run) expected average cost per unit time.

1.

$$\begin{vmatrix} 0.6 & 0.4 \\ 0.4 & 0.6 \end{vmatrix}$$

$$p_{11} = P(D=0) + P(D=2) + P(D=4) = \frac{3}{5} = 0.6.$$

$$p_{21} = P(D=1) + P(D=3) = \frac{2}{5} = 0.4.$$

2.

$$\Pi_1 = \Pi_2 = 0.5.$$

3.

$$k(1) = E(C(1, D)) =$$

$$1P(D=0) + 4P(D=1) + (4+4)P(D=2) + (8+6)P(D=3) + (12+6)P(D=4) =$$

$$\frac{1}{5}(1+4+8+14+18) = \frac{45}{5} = 9.$$

$$k(2) = E(C(2, D)) =$$

$$2P(D=0) + 1P(D=1) + 4P(D=2) + (4+4)P(D=3) + (8+6)P(D=4) =$$

$$\frac{1}{5}(2+1+4+8+14) = \frac{29}{5}.$$

$$\frac{1}{2}\left(\frac{45}{5}\right) + \frac{1}{2}\left(\frac{29}{5}\right) = \frac{74}{10} = 7.4.$$

Problem 23, part c only: Consider the following gambler's ruin problem. A gambler bets one unit on each play of a game. She has a probability p of winning and $q = 1-p$ of losing. She will continue to play until she goes broke or nets a fortune of T units. Let X_n denote the gambler's fortune on the $n-th$ play of the game. Then,

$$X_{n+1} \begin{cases} X_n + 1, & \text{with probability } p. \\ X_n - 1, & \text{with probability } q = 1-p \end{cases} \tag{5.4}$$

for $0 < X_n < T$. $X_{n+1} = X_n$, for $X_n = 0$, or T. X_n is a Markov chain. Assume that successive plays of the game are independent and that the gambler has an initial fortune of X_0.

1. Determine the one-step transition matrix of the Markov chain.

2. Find the classes of the Markov chain.
3. Let $T = 3$ and $p = 0.3$. Find $f_{10}, f_{1T}, f_{20}, f_{2T}$.
4. Let $T = 3$ and $p = 0.7$. Find $f_{10}, f_{1T}, f_{20}, f_{2T}$.

What can you conclude from (c) and (d)?

1. $$\begin{vmatrix} 0 & 1 & 2 & . & . & . & \text{T-1} & \text{T} \\ 1 & 0 & & & & & & \\ q & 0 & p & & & & & \\ & q & 0 & p & & & & \\ & & . & . & . & & & \\ & & & . & . & . & & \\ & & & & . & . & . & \\ & & & & & q & 0 & p \\ & & & & & & 0 & 1 \end{vmatrix}$$

2. {0} absorbing, {1,...,T-1} transient, {T} absorbing.

3. $$\begin{vmatrix} 1 & 0 & 0 & 0 \\ 0.7 & 0 & 0.3 & 0 \\ 0 & 0.7 & 0 & 0.3 \\ 0 & 0 & 0 & 1 \end{vmatrix}$$

$$f_{10} = 0.7 + 0.3 f_{20},\ f_{20} = 0.7 f_{10}.$$

Using substitution, the following values are obtained.

$$f_{10} = \frac{70}{79},\ f_{20} = \frac{49}{79},\ f_{13} = 0.3 f_{23},\ f_{23} = 0.7 f_{13} + 0.3.$$

Using substitution, the following values are obtained.

$$f_{13} = \frac{9}{79},\ f_{23} = \frac{30}{79}.$$

4.

$$\begin{vmatrix} 1 & 0 & 0 & 0 \\ 0.3 & 0 & 0.7 & 0 \\ 0 & 0.3 & 0 & 0.7 \\ 0 & 0 & 0 & 1 \end{vmatrix}$$

$$f_{10} = 0.3 + 0.7 f_{20},\ f_{20} = 0.3 f_{10}.$$

Using substitution, the following values are obtained.

$$f_{10} = \frac{30}{79},\ f_{20} = \frac{9}{79},\ f_{13} = 0.7 f_{23},\ f_{23} = 0.3 f_{13} + 0.7.$$

Using substitution, the following values are obtained.

$$f_{13} = \frac{49}{79},\ f_{23} = \frac{70}{79}.$$

The likelihood of losing will decrease as the probability of winning...

Problem 24: A video recorder manufacturer is so certain of its quality control that it is offering a complete replacement warranty if the set fails within two years. Based upon compiled data, the company has noted that only 1 percent of its recorders fail during the first year and 5 percent fail during the second year. The warranty does not cover replaced recorders.

1. Formulate this problem as a Markov chain and determine the transition matrix.
2. Find the probability that the manufacturer will have to honor the warranty.

1. States: 0: recorder replaced, 1: recorder in first year, 2: recorder in second year, 3: recorder two or more years old.

$$\begin{array}{c|cccc|} 0 & 1 & 0 & 0 & 0 \\ 1 & 0.01 & 0 & 0.99 & 0 \\ 2 & 0.05 & 0 & 0 & 0.95 \\ 3 & 0 & 0 & 0 & 1 \end{array}$$

2. $f_{10} = 0.10 + 0.99 f_{20}$, $f_{20} = 0.05$. Using substitution, $f_{10} = 0.0595$, which is the probability of honoring the warranty.

5.2.8 Summary

- Markov Property,

$$P(x_n = j | x_0 = i_0, x_2 = i_1, ..., x_{n-1} = k) = P(x_n = j | x_{n-1} = k).$$

- Stationary Markov Chain,

$$\forall n, j, k, P(x_{n+1} = j | x_n = k).$$

- Step Transition Matrix,

$$\mathrm{IP}^{(n)} = \mathrm{IP}^n.$$

- Communicating Class of States($i \leftrightarrow j$), If i communicates with j and j communicates with k, then $i \leftrightarrow k$.
- Closed Class, a set of states is closed if no state in T leads to a state outside of T.
- Recurrent, state i is recurrent if the probability of returning to state i given it is in state i is 1.
- Transient, states are not recurrent.
- E(number of steps), Let T_{ij} be i number of states until state j is reached. $\mu_{ij} = E(T_{ij})$,

$$\mu_{ij} = 1 + \sum_{k \neq j} P_{ik} \mu_{kj}, \forall i.$$

  Also called E(recurrent time).
- steady State Equation, use the following formula in Gaussian elimination.

$$\sum_{i=0}^{n} \pi_i = 1.$$

- Aperiodic, state j has a period of 1. For any recurrent state,

$$LCD(n : P_{ij}^{(n)}\ 0)$$

  is the period.

- Stationary Solution, exists for chains that are irreductible but not aperiodic. there is no steady state solution.

- Costs, Fixed costs are $\sum_{k=0}^{n} C(k)\Pi_k$, Random costs are $\sum_{j=0}^{n} k(j)\Pi_j =$

$$\sum_{k=0}^{n} E(C(k,D))\Pi_k.$$

- Probability of Reaching an Absorbing State, $f_{ir} = P(x_n = r \text{ for some } n | x_0 = i)$.

$$_{ik} = \sum_{j=0}^{m} P_{ij} f_{jk}, \forall i.$$

$$f_{kk} = 1, f_{ik} = 0$$

for recurrent states.

5.3 Queuing Theory

5.3.1 Memoryless Property

The *exponential* density is, $f(t) = \alpha e^{-\alpha t}, 0 \leq t$. The cumulative distribution is, $F(t) = P(x \leq t) = 1 - e^{-\alpha t}$ for $0 \leq t$ or $P(x > t) = e^{-\alpha t}$, for $0 \leq t$. $E(x) = \frac{1}{\alpha}$, and $\sigma_x^2 = \frac{1}{\alpha^2}$. The *Poisson* distribution is, $f(n) = P(y = n) = e^{-\alpha} \frac{\alpha^n}{n!}$ for n=0,1,2,3,.... The cumulative distribution function is, $F(N) = P(y \leq N) = e^{-\alpha} \sum_{n=0}^{N} \frac{\alpha^n}{n!}$. N(t) is a random variable for each $t \geq 0$. Each N(t) takes values in the non-negative integers. The assumptions are as follow:

1. N(0) = 0.

2. N(t+s) - N(s) has a Poisson distribution with a mean $\lambda\Pi$. λ is termed the mean rate per unit of time. $P(N(t+s) - N(s) = n) = \frac{e^{-\lambda t}(\lambda t)^n}{n!}$, for n = 0,1,2,....

3. If $0 \leq t_1, < t_2 < t_x < ... < t_n$ then $N(t_1) - N(0), N(t_2) - N(t_1), N(t_3) - N(t_2), ..., N(t_n) - N(t_{n-1})$ are independent random variables. Then, N(t) is a *Poisson process.*

Let T be the time until the first observation(event). T is a random variable whose values are non-negative. The cumulative distribution function is $F_T(t) = P(T \leq t). = 1 - P(T > t) = 1 - P(N(t) = 0) = 1 - P(N(t) - N(0) = 0) = 1 - e^{-\lambda t}$. The probability density function is

$$f_T(t) = F_T'(t) = \lambda E^{-\lambda t}, T \geq 0.$$

Let T_i be the time from the i-1st event until the i-2nd event(called the ith interarrival). Then,

$$P(T > t - s | T > s) = \frac{P(T > t + s)}{P(T > s)} = \frac{e^{-\lambda(t+s)}}{e^{-\lambda s}} = e^{-\lambda t} = P(T > t).$$

That is called the *memoryless property.*

5.3.2 Poisson Processes

Let N(t) be a Poisson process. Then,

$$P(N(t+s)-N(s)=j)=\frac{e^{-\lambda t}(\lambda t)^j}{j!}, j=0,1,2,....$$

T time between any two events has an exponential density $\lambda e^{-\lambda t}$.

$$F_T(t)=p(T\le t)=1-e^{-\lambda t},$$

or

$$P(T>t)=e^{-\lambda t}.$$

Let $T_1, T_2, T_3, ..., T_n$ be independent exponential random variables such that $E(T_i)=\frac{1}{\alpha_i}$. Let $m=\min(T_1,$ T_2, ..., $T_i)$, $1\le i\le m$.

Example: Let A, B, and C be airlines. Planes for A arrive as a Poisson process with mean rate q. Assume processes are independent. Let N(t) be the number of planes that arrive in time t. Let T_A, T_B, T_C be the time until the next plane of A, B, C arrives. Let T be the time until the next plane arrives. $T=\min(T_A,T_B,T_C)$. Prove that T is exponential. $1-F_m(t)=1-P(M\le t)=P(m\ge t)=P(\cap_{i=1}^m T_i>t)=\Pi_{i=1}^m P(T_i>t)=\Pi_{i=1}^m e^{-\alpha_i t}=e^{-\alpha_1+-\alpha_2+...+-\alpha_m t}=e^{-(\sum_{i=1}^m\alpha_i)t}$. $F_m(t)=1-e^{-(\sum_{i=1}^m\alpha_i)t}$. m has an exponential distribution with mean $\frac{1}{\sum_{i=1}^m\alpha_i}$. So, $\frac{1}{a+b+c}$ is the exponential mean. Thus $N(t)$ is a Poisson process with mean rate, $a+b+c$. Let N(t) be a Poisson process with mean rate λ and let T_n be the time at the n-th event. T_i is the time between the ith event and $i+1$-st event. See Figure 5.14.

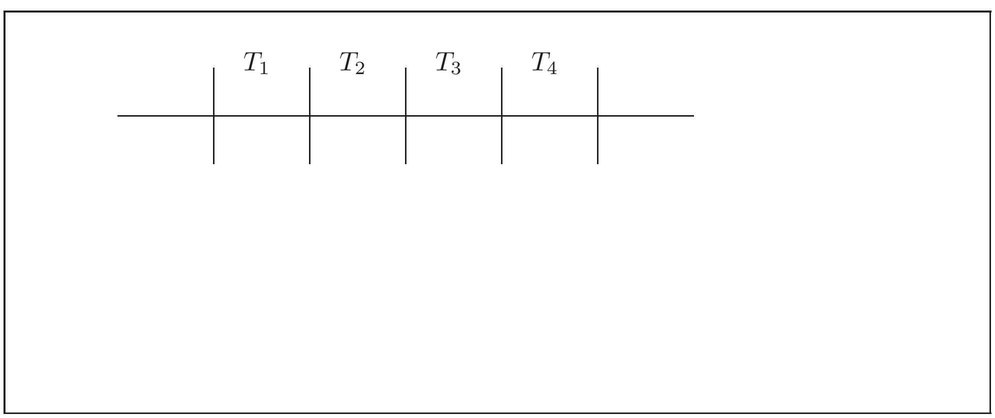


Figure 5.14:

So, $T_n=\sum_{i=1}^n T_i$. Each T_i is exponential with mean $\frac{1}{\lambda}$. $F_{T_n}(t)=P(T\le t)=1-P(T_n>t)=1-P(N(t)\le n-1)=1-\sum_{i=0}^{n-1}=\frac{e^{-\lambda t}(\lambda t)^i}{i!}$. Using algebra, the density is

$$f_{T_n}(t)=F'_{T_n}(t)=-\left[\sum_{i=1}^{n-1}e^{-\lambda t}\frac{(\lambda T)^i}{i!}\right]'-[e^{-\lambda t}]'=-\sum_{i=1}^{n-1}\left[-\lambda e^{-\lambda t}\frac{(\lambda t)^i}{i!}+\frac{e^{-\lambda t}i(\lambda t)^{i-1}\lambda}{i!}\right]+\lambda e^{-\lambda t}=$$

$$\left[\lambda e^{-\lambda t}\sum_{i=1}^{n-1}\frac{(\lambda t)^i}{i!}\right]-\left[\lambda e^{-\lambda t}\sum_{i=1}^{n-1}\frac{(\lambda t)^{i-1}}{(i-1)!}\right]=...=\lambda e^{-\lambda t}\left[\frac{\lambda^n t^{n-1}}{(n-1)!}\right], 0\le t.$$

The last equation is called the *gamma* density. This particular form is called the *Erlang* density.

$$E(T_n) = E\left(\sum_{i=1}^{n} T_i\right) = \sum_{i=1}^{n} E(T_i) = \sum_{i=1}^{n} \frac{1}{\lambda} = \frac{n}{\lambda}.$$

$$\sigma^2_{T_n} = \sigma^2_{\sum_{i=1}^{n} T_i} = \sigma^2_{T_i} = \sum_{i=1}^{n} \frac{1}{\lambda^2} = \frac{n}{\lambda^2}.$$

5.3.3 Queuing Notation and Variables

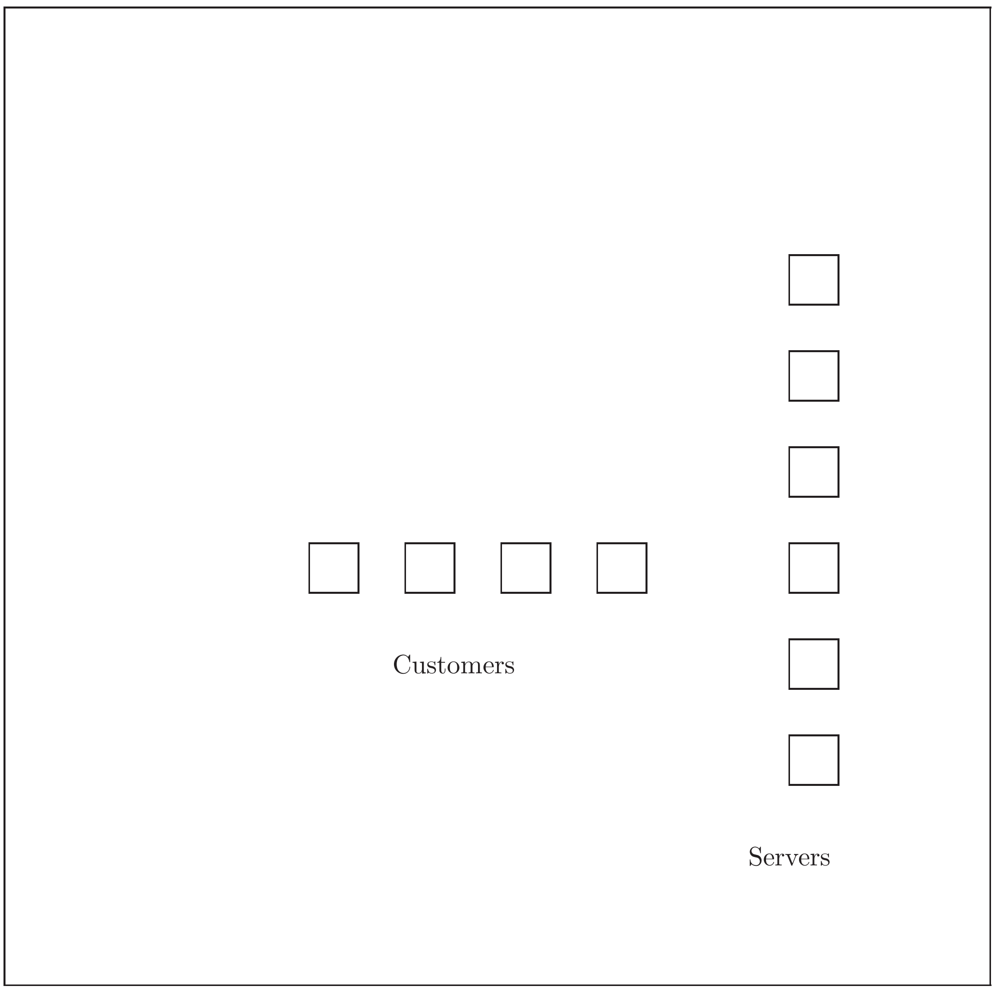


Figure 5.15: A General Queue

See Figure 5.15 for a general queue setup. To describe the queue, the following notation is used:

- M is a Poisson process of how customers arrive and customers leave.
- D means arrivals are deterministic.
- E_k means the arrivals/departures are Erlang with parameter k. k is called the *degrees of freedom.*
- G means arrivals/departures are general.

- GI means arrivals/departures are general independent.

The notation used for queues is as follow: Arrival distribution/service time distribution/number of servers/max system size/service discipline.

Example: $M/E_3/5/100/FIFO$. Everything we will do in Queuing theory is *steady state.* Some of the variables used follows.

- N is the number of customers in the system(i.e. the system size).
- $L = E(N)$ is the expected system size.
- W is the waiting time of customers.
- $W = E(W)$ is the expected waiting time in the system.
- N_q is the number of customers in the queue.
- $L_q = E(N_q)$ is the expected queue length.
- W_q is the waiting time in queue.
- $W_q = E(W_q)$ is the expected waiting time in queue.

L, L_q, W, W_q are called *measures of effectiveness.* P_n is the steady state probability of there being n customers in the system. λ is the arrival rate. $L = \lambda W$ is called *Little's Formula.* The birth and death process N(t) has the following characteristics:

1. Time short interval N(t) goes up by one or down by one or does not change.
2. Time until the next birth is exponential with mean $\frac{1}{\lambda_n}$ where n is the current value of N.
3. Time until the next death is exponential with mean $\frac{1}{\mu_n}$.

States are the number of customers. See Figure 5.16.
The probability of being in state 3 is $P_2\lambda + P_4\mu_4 = P_3$ which is the rate of leaving state 3. The rate of coming into state 3 is $P_3\mu_3 + P_3\lambda_3$. Therefore the *balanced equation* is $P_2\lambda_2 + P_4\mu_4 = P_3\mu_3 + P_3\lambda_3$. In general,

$$\mu_1 P_1 = \lambda_0 P_0,$$

$$\lambda_0 P_0 + \mu_2 P_2 = \lambda_1 P_1 + \mu_1 P_1,$$

$$...$$

$$\lambda_{n-1} P_{n-1} + \mu_{n+1} P_{n+1} = (\lambda_n + \mu_n) P_n.$$

Solving the above equations, we get:

$$P_1 = \frac{\lambda_0 P_0}{\mu_1}.$$

$$P_2 = \frac{1}{\mu_2}((\lambda_1 + \mu_1)P_1 - \lambda_0 P_0).$$

$$P_n = \frac{\lambda_0 \lambda_1 ... \lambda_{n-1}}{\mu_1 \mu_2 ... \mu_n} P_0.$$

Let $C_n = \frac{\lambda_0 \lambda_1 ... \lambda_{n-1}}{\mu_1 \mu_2 ... \mu_n}$. Then, $P_n = C_n P_0$. $1 = \sum_{n=0}^{\infty} P_n = \sum_{n=0}^{\infty} C_n P_0 = P_0 \sum_{n=0}^{\infty} C_n$. Then, $P_0 = \frac{1}{\sum_{n=0}^{\infty} C_n}$. Then, $P_n = \frac{C_n}{\sum_{j=0}^{\infty} C_j}$.

Example: $M/M/1/\infty/FIFO$. $\lambda_n = \lambda$, $\mu_n = \mu$. Then, $C_n = \frac{\lambda^n}{\mu^n} = (\frac{\lambda}{\mu})^n$. Let $\rho = \frac{\lambda}{\mu}$. Then, $P_0 = \frac{1}{\sum_{n=0}^{\infty} \rho^n} = \frac{1}{\frac{1}{1-\rho}} = 1 - \rho, \lambda < \mu$. $P_n = \rho^n(1-\rho)$. ρ is the probability that the server is busy. It is called the *utilization factor.* $P(N \geq 1) = 1 - P(N = 0) = 1 - P_0 = 1 - (1 - \rho) = \rho$.

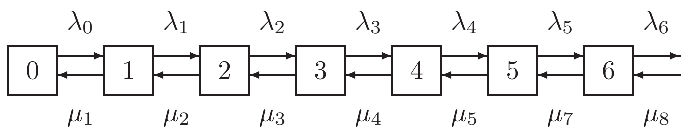


Figure 5.16: Customers

5.3.4 Priority Queuing

Consider an $M/M/s/\infty$ queue with three types of customers. Type 1 has highest priority, type 2, and type 3 have lowest priority. Each type j arrives as a Poisson process with mean rate λ_j. Taken all together, arriving customers for a Poisson process with mean rate $\lambda = \lambda_1 + \lambda_2 + \lambda_3$. There are two types of priorities: 1) nonpremptive where customers cannot loose service, and 2) preemptive where the server can be taken away from the customer and given to a higher priority customer. Compute W_1 for the highest priority, W_2 for the next highest priority, and W_3 for the lowest priority. In a non-preemptive priority discipline, assume all service times are the same. $\lambda \leq s\mu$ must be true to approach steady state.

Example: Two types of calls come to the sheriff's office: critical and routine. Two deputies answer the phones. Critical calls come as a Poisson process with a mean rate of 1 every 3 hours. Routine calls come at a rate of 2 per hour. The time needed to handle a call is exponential with a mean rate of 45 minutes. Find W_{q1}, and W_{q2}.

$$\lambda_1 = \frac{1 \text{ call}}{3 \text{ hr}},\ \lambda_2 = \frac{2 \text{ calls}}{\text{hr}},\ \lambda = \lambda_1 + \lambda_2 = \frac{7 \text{ calls}}{3 \text{ hrs}}.$$

$\frac{1}{\mu} = \frac{3}{4}$. Therefore, $\mu = \frac{4}{3 \text{ hrs}}$. $s = 2$. Therefore, $S\mu = 2\frac{4}{3} = \frac{8}{3} > \frac{7}{3} = \lambda$. Therefore, a steady state exists. Reference page 637 in the text book for the formulas.

$$B_0 = 1,\ B_1 = 1 - \frac{\lambda_1}{s\mu} = 1 - \frac{\frac{1}{3}}{\frac{8}{3}} = \frac{7}{8},\ B_2 = 1 - \frac{\lambda_1 + \lambda_2}{s\mu} = 1 - \frac{\frac{7}{3}}{\frac{8}{3}} = 1 - \frac{7}{8} = \frac{1}{8}.$$

$$A = s!\left(\frac{s\mu - \lambda}{rs}\right)\sum_{j=0}^{s-1}\frac{r^j}{j!} + s\mu,\ A = 2\left(\frac{\frac{8}{3} - \frac{7}{3}}{(\frac{7}{4})^2}(1 + \frac{7}{4}) + \frac{8}{3}\right) = 3.2653,\ W_1 = \frac{1}{AB_0B_1} + \frac{1}{\mu}.$$

We want W_{q1}.

$$W_{q1} = W_1 - \frac{1}{\mu} = \frac{1}{AB_0B_1} = \frac{1}{(3.2653)(1)(\frac{7}{8})}.$$

which is equal to 0.35 hours or 21 minutes.

$$W_2 = \frac{1}{AB_1B_2} + \frac{1}{\mu}, \, W_{q2} = W_2 - \frac{1}{\mu} = \frac{1}{(3.2653)(\frac{7}{8})(\frac{1}{8})} = 2.8hrs.$$

Next, use the preemptive priority on the same example. For critical calls, we have an M/M/2 queue with arrival rate $\lambda_1 = \frac{1}{3}$, and a service rate $\frac{1}{\mu} = \frac{3}{4}$. $W_{q1} = \frac{1}{84}hrs$ or 43 seconds. There is a tremendous improvement on W_{q1}. Consider the queue overall. $\lambda = \frac{7}{3}$, $\mu = \frac{4}{3}$, M/M/s where s=2.

$$W_{q_{12}} = \frac{49}{20} = 2.45, \, W_{q_{12}} = \left(\frac{\frac{1}{3}}{\frac{7}{3}}\right) W_{q1} + \left(\frac{2}{\frac{7}{3}}\right) W_{q2} = 2.45 = \left(\frac{1}{7}\right)\left(\frac{1}{84}\right) + \frac{6}{7} W_{q2},$$

$$W_{q2} = 2.8563 \text{ hrs} = 2 \text{ hrs}, 5 \text{ mins}.$$

5.3.5 M/M/s Queue and Jackson Network

$M/M/s$ queue of customers leaving. See Figure 5.17. There is an infinite capacity and an infinite population.

Look at customers leaving $\Rightarrow s\lambda$. Look at customers entering $\Rightarrow s\mu$. $M/M/s/\infty/\infty$. Look at service queue. See Figure 5.18.

These are three problems of $M/M/s/\infty/\infty$. $L = L_1 + L_2 + L_3$. $W = W_1 + W_2 + W_3$. The joint pmf is,

$$f(n_1, n_2, n_3) = P(N_1 = n_1, N_2 = n_2, N_3 = n_3) = P(N_1 = n_1)P(N_2 = n_2)P(N_3 = n_3).$$

The Jackson Network

See Figure 5.19 for a Jackson Network.

At station 1, customers arrive as a Poisson process with mean rate λ_1.

$$\lambda_1 = \alpha_1 + p_{21}\lambda_2 + p_{31}\lambda_3, \, \lambda_2 = \alpha_2 + p_{12}\lambda_1 + p_{32}\lambda_3, \, \lambda_3 = \alpha_3 + p_{13}\lambda_1 + p_{23}\lambda_2.$$

Solve the system for $\lambda_i's$. Each server is an M/M/s server with arrivals of λ_i. $L = L_1 + L_2 + L_3$. $W = \frac{L}{\alpha_1 + \alpha_2 + \alpha_3}$.

Example: A railroad has a system of 4 yards. Box cars can enter the system at any yard. See Figure 5.20.

yard	1	2	3	4
number per day	50	100	75	210

i is the starting yard and j is the ending yard. i is horizontal in the following table and j is vertical.

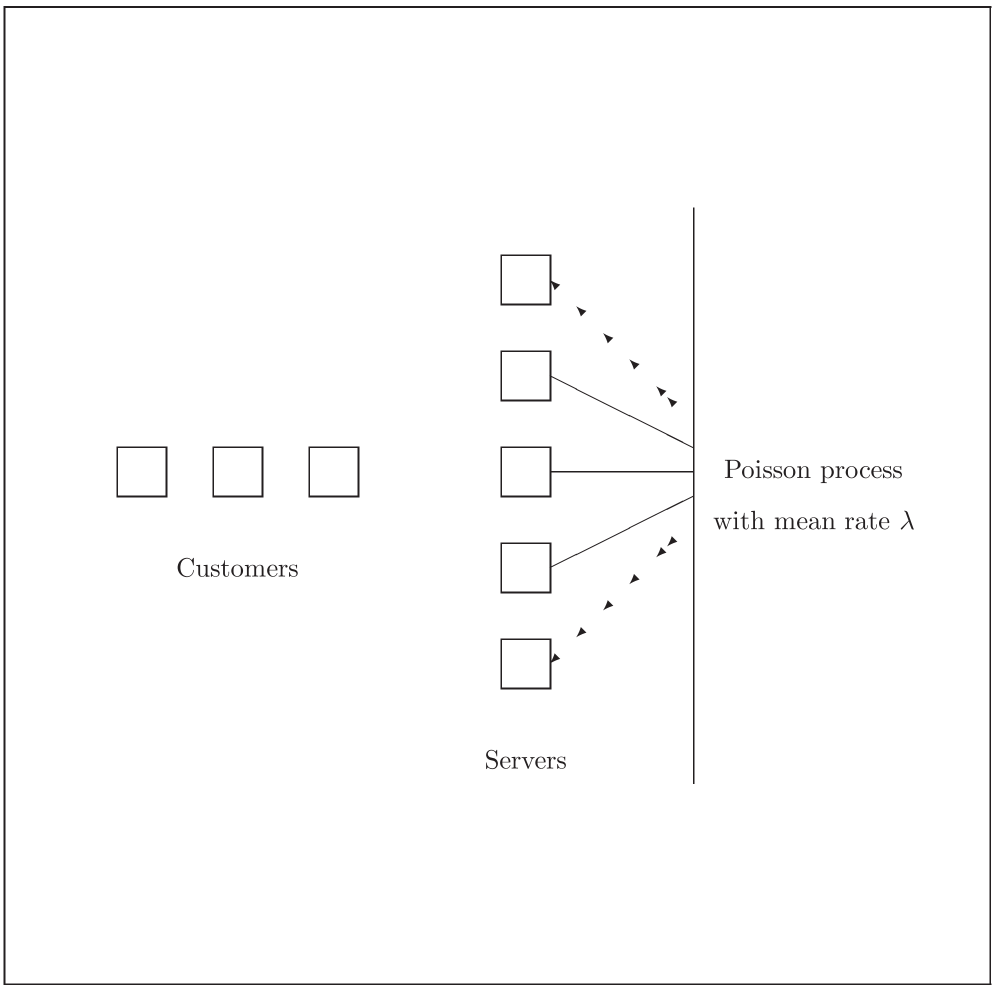
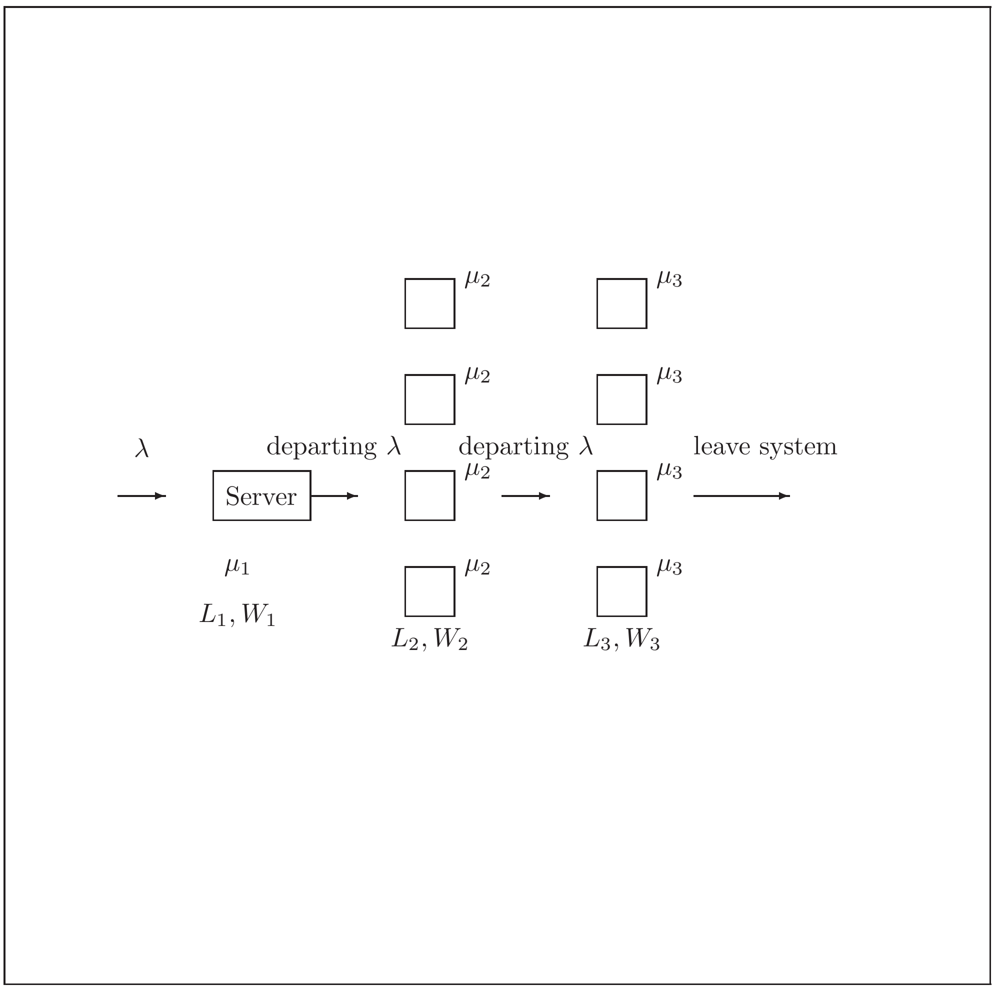


Figure 5.17:



λ
Server
μ_1
L_1, W_1
departing λ
μ_2
μ_2
μ_2
μ_2
L_2, W_2
departing λ
μ_3
μ_3
μ_3
μ_3
L_3, W_3
leave system

Figure 5.18:

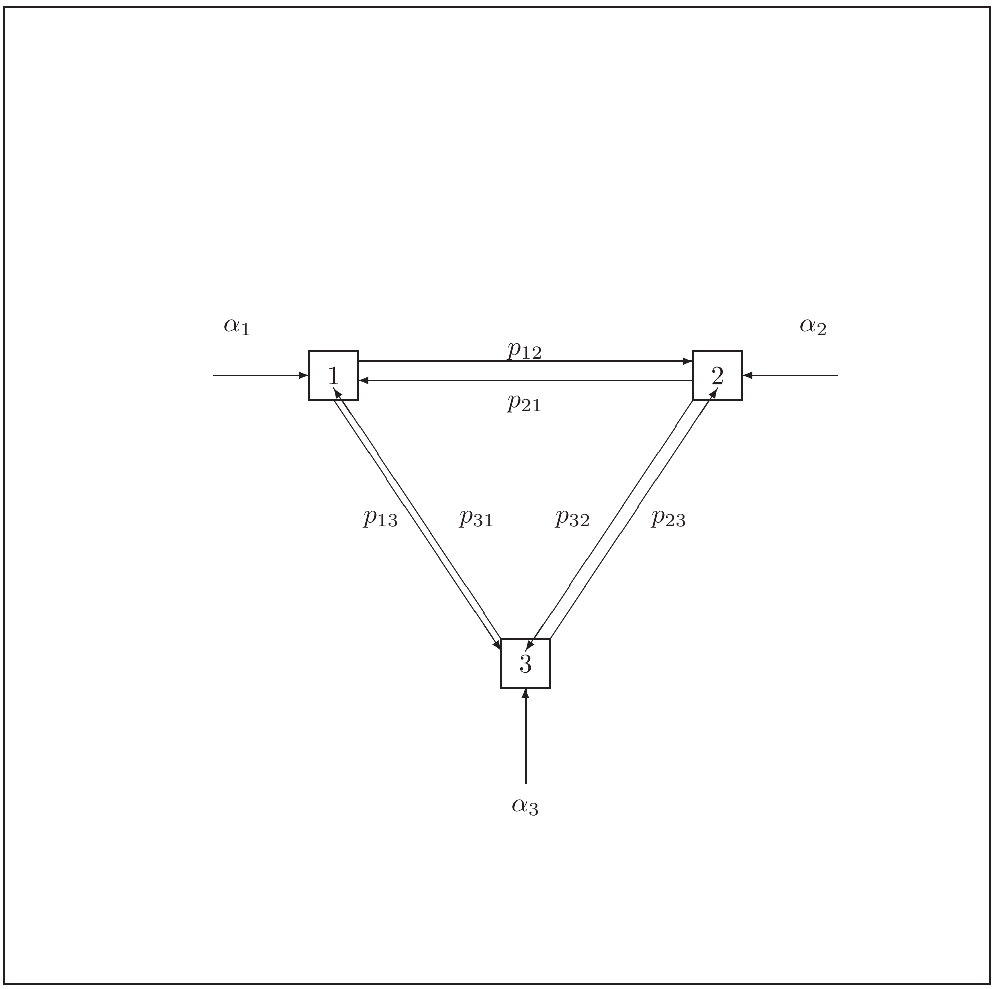


Figure 5.19: A Jackson Network

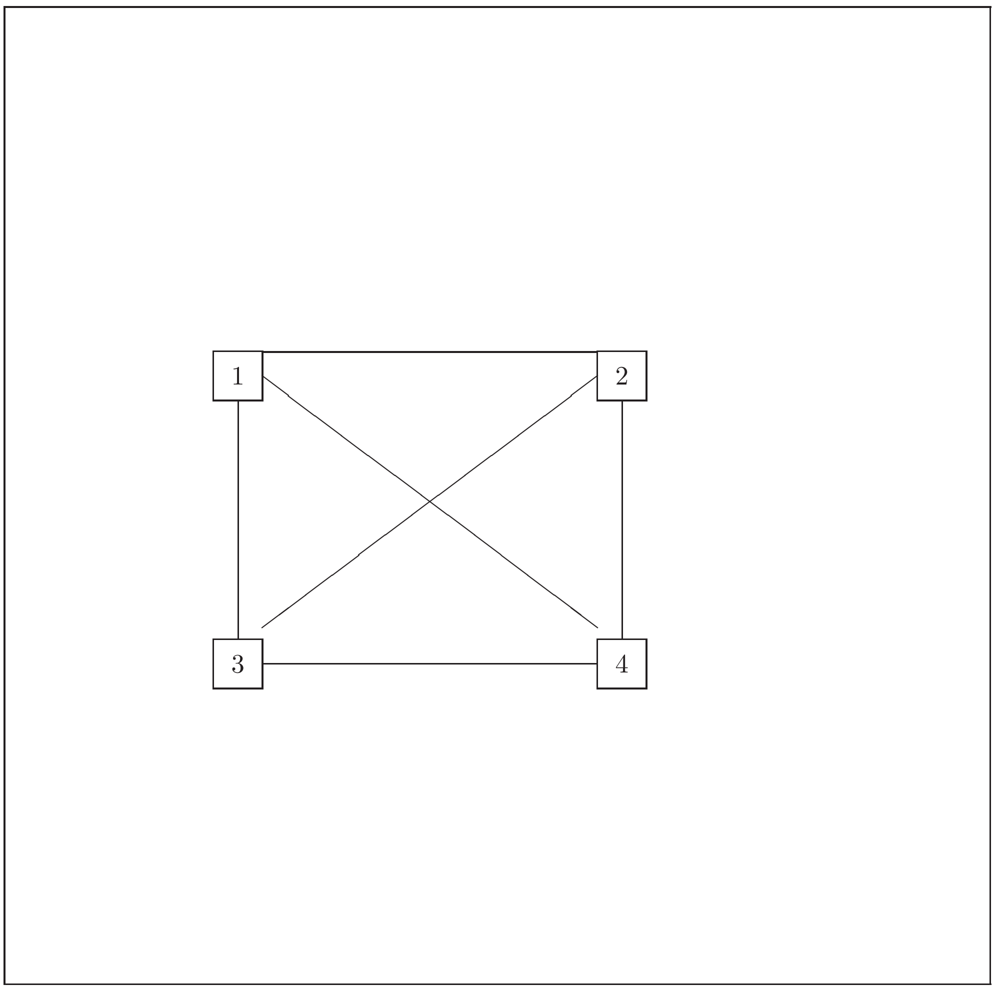


Figure 5.20:

i/j	1	2	3	4
1	0	0.4	0	0.3
2	0.3	0	0.6	0.1
3	0	0.3	0	0.2
4	0.5	0.1	0.1	0

There is a probability that box cars can leave the system.

$$\lambda_1 = 50 + 0.4\lambda_2 + 0.3\lambda_4,\ \lambda_2 = 100 + 0.3\lambda_1 + 0.6\lambda_3 + 0.1\lambda_4,$$

$$\lambda_3 = 75 + 0.3\lambda_2 + 0.2\lambda_4,\ \lambda_4 = 210 + 0.5\lambda_1 + 0.1\lambda_2 + 0.1\lambda_3.$$

Solve the system so that,

$$\lambda_1 = 363.25,\ \lambda_2 = 434.4579,\ \lambda_3 = 298.3184,\ \lambda_4 = 464.905.$$

Assume that $\mu_1 = 375, \mu_2 = 440, \mu_3 = 450, \mu_4 = 468$. Then,

$$L_1 = 30.9275,\ L_2 = 78.3924,\ L_3 = 1.9667,\ L_4 = 150.2092.$$

L_2 and L_4 are the most trouble. Look at the number of cars greater than the yard capacity. What is $P(N_2 > 300)$? $P(N_2 > 300) = 0.022$, $P(N_4 > 250) = 0.1891$. $L = L_1 + L_2 + L_3 + L_4 = 261.4958$. $W = \frac{L}{50+100+75+210} = 0.6011$, or approximately $\frac{1}{2}$ day. The costs depend on the number of customers in the system and how long customers have to wait. Our measures of effectiveness are averages: L, W, L_q, W_q, and are usually linear. For non-linear measures, we must get the distributions of the measures.

Example: $F_W(t) = P(W \leq t)$.

5.3.6 M/G/1 Model

Some notes are missing from the previous lecture on M/G/1 models. λ is the parameter for input process(mean arrivals in unit time). μ is 1/(mean service time). σ^2 is the variance of the service time. $L_q = \frac{\lambda\sigma^2+\rho^2}{2(1-\rho)}$. Reference page 629 in the text book. For the M/M/1 model, derivation of Ł$_q = \frac{\lambda^2\frac{1}{\mu^2}+\rho^2}{2(1-\rho)}$. $\frac{2\rho^2}{2(1-\rho)} = \frac{\rho^2}{1-\rho} = \frac{\lambda^2}{\mu(\mu-\lambda)}$. $W_q = \frac{L_q}{\lambda}$. $W = W_q +$ E (service time) $= W_q + \frac{1}{\mu}$. $L = \lambda W = \lambda W_q + \frac{\lambda}{\mu} = L_q + \frac{\lambda}{\mu}$.

Example: Reading requires s minutes where s is uniform on [6,16]. Computation check k is exponential with mean 4. Arrivals are Poisson with a mean rate of 3 per hour. s and k are independent. What is the expected time from the arrival of a return until she is finished with it? M/G/1 queue with two random variables s, and k. $\lambda = 3$, $\frac{1}{\mu} =$ E(s+k) $=$ E(s) $+$ E(k) $= \frac{16+6}{2} + 4 = 11 + 4 = 15$ minutes. $\frac{1}{\mu} = \frac{1}{4}$ hours. Therefore $\mu = 4$. $\sigma^2_{s+k} = \sigma^2_s + \sigma^2_k = \frac{(16-6)^2}{12} + 16 = \frac{73}{3}$. The question asks for W. $\rho = \frac{\lambda}{\mu} = \frac{3}{4}$. $\lambda = \frac{1}{20}$ per minute. $L_q = \frac{\frac{1}{400}\frac{73}{3}+\frac{9}{16}}{2(\frac{1}{4})} = 1.2467$. $W = W_q + \frac{1}{\mu} = \frac{L_q}{\lambda} + \frac{1}{\mu} = 20(1.25) + \frac{15}{1} = 39.933$.

Example: $\lambda = \frac{1}{3}$. A single team works on one camel at a time. There are five processes, killing-bleeding, scolding, gritting, shimming, cattling up. Each process is exponential time with mean of 35 minutes. The times are independent and must be finished before the next on starts. What is the average number waiting in the pen outside?

This is an $M/E_s/1$ model. An Erlang model is where there is a sum of independent exponentials. $\frac{1}{\mu} = \frac{35}{12}$. $\mu = \frac{12}{35}$. $\sigma^2 = 5(\frac{49}{144}) = \frac{245}{144}$. The question asks for L_q. Therefore,

$$\rho = \frac{\frac{1}{3}}{\frac{12}{35}} = \frac{35}{36}.$$

$L_q = 20.4167$. Suppose a second team is added. What will be the wealth of adding a second team? This is a $M/E_5/2$ model. We cannot calculate L with formula. Use the graph on page 633 in the text book. $\rho = \frac{\lambda}{s\mu}$, $k = 5$, $\rho = \frac{\frac{1}{3}}{2(\frac{12}{35})} = \frac{35}{72} = 0.486$. $L \approx 1.2$ from reading the table on page 633. $W = W_q + \frac{1}{\mu} = \lambda W = \lambda W_q + \frac{\lambda}{\mu}$. $L = L_q + \frac{\lambda}{\mu} = 1.2\frac{35}{36} = 0.228$.

5.3.7 Homework and Answers

Do problems 5, 7, 11, 12, 17, 21, 23, 24, 27, 29, 35, 36, 38, 45, 46, 47 in the text book.

Problem 5: A service station has one gasoline pump. Cars wanting gasoline arrive according to a *Poisson* process at a mean rate of 15 per hour. However, if the pump already is being used, then potential customers may *balk* (drive to another service station). In particular, if there are n cars already at the service station, the probability that an arriving potential customer will balk is $\frac{n}{3}$ for $n = 1, 2, 3$. The time required to service a car has an *exponential* distribution with mean of 4 minutes.

1. Construct the rate diagram for this Queuing system.
2. Develop the balanced equations.
3. Solve these equations to find the steady-state probability distribution of the number of cars at the gas station. Verify that this solution is the same as that given by the general solution for the *birth-and-death process.*
4. Find the expected waiting time(including service time) for those cars that stay.

Given: $\lambda = (\frac{15cars}{hr})(\frac{1hr}{60min}) = \frac{0.25cars}{min}$.

1. See Figure 5.21.
2. $$\mu P_0 = \mu P_1,\ (\mu+\lambda)P_1 = \lambda P_0 + \mu P_2,\ (\mu+\lambda)P_2 = \lambda P_1 + \mu P_3,\ ...,\ (\mu+\lambda)P_{n-1} = \lambda P_{n-2} + \mu P_n.$$
3. $$(0.25)P_0 = 4P_1,\ P_0 = \frac{4P_1}{0.25}.$$
   Therefore,
   $$P_1 = \frac{0.25}{4}P_0 = 0.0625P_0,\ (4+0.25)P_1 = 0.25P_0 + 4P_2,$$
   $$P_2 = \frac{(4+0.25)P_1 - 0.25P_0}{4} = 0.0039062P_0,\ C_n = \frac{(0.25)^{n-1}}{4^n},$$
   Therefore,
   $$P_n = C_nP_0 = \frac{0.25^{n-1}}{4^n}\rho_0.$$
4. $E(W) = 6.3529$ minutes.

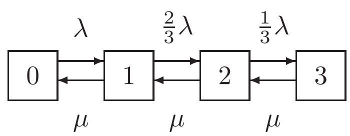


Figure 5.21:

Problem 7: A certain small grocery store has a single checkout stand with a full-time cashier. Customers arrive at the stand 'randomly'(i.e. a Poisson input process) at a mean rate of 30 per hour. When there is only one customer at the stand, he is processed by the cashier alone, with an expected service time of 1.5 minutes. However, the stock boy has been given standard instructions that whenever there is more than one customer at the stand, he is to help the cashier by bagging the groceries. this help reduces the expected time required to process a customer to 1 minute. In both cases, the service-time distribution is exponential.

1. Construct the rate diagram for this Queuing system.
2. What is the steady-state probability distribution of the number of customers at the checkout stand?
3. Derive L for this system. Use this information to determine L_q, W, and W_q.

Given: $\lambda = \frac{30 \text{ customers}}{\text{hr}} \frac{1 \text{ hr}}{60 \text{ min}} = \frac{1 \text{ customer}}{2 \text{ min}}$.

1. See Figure 5.22.
2.

$$P_1 \mu_A = P_0 \lambda,$$

$$\lambda P_0 + \mu_H P_2 = \lambda P_1 + \mu_A P_1,$$

$$\lambda P_1 + \mu_H P_3 = \mu_H P_2 + \lambda P_3,$$

...

...

...

$$\lambda P_{n-1} + \mu_H P_{n+1} = \mu_H P_N + \lambda P_{n+1}.$$

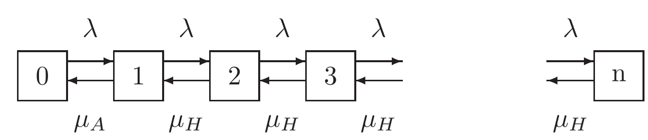


Figure 5.22:

3.

$$P_1 = \frac{P_0}{3},\ P_2 = 0.5P_0,\ P_n = \frac{2(\frac{1}{2})^n}{3},\ C_n = \frac{(\frac{1}{2})^n}{1.5},\ P_0 = \frac{1}{1+\frac{1}{2}+\frac{1}{4}+\frac{1}{8}+\ldots}.$$

$$S_n - \frac{S_n}{2} = \frac{1}{2} + \left(\frac{1}{2}\right)^{n+1},\ \lim_{n\to\infty} S_n = 1.$$

Therefore,

$$P_0 = \frac{1}{1+1.5} = 0.4,\ L = 0 + \frac{\lambda}{\mu_A} + \sum_{n=2}^{\infty} n\rho^n, \rho = \frac{\lambda}{\mu_H}.$$

Problem 11: A bank employs four tellers to serve its customers. Customers arrive according to a Poisson process at a mean rate of three per minute. If a customer finds all tellers busy, he joins a queue that is serviced by all tellers; that is, there are no lines in front of each teller, but rather one line waiting for the first available teller. The transaction time between the teller and customer has an exponential distribution with a mean of 1 minute.

1. Construct the rate diagram for this Queuing system.
2. Find the steady-state probability distribution of the number of customers in the bank.
3. Find L_q, W_q, W, and L.

Given: $\lambda = \frac{3 \text{ customers}}{1 \text{ min}}$, and $\mu = 1 \text{ min} = \frac{1}{1 \text{ min}} = 1.$

1. See Figure 5.23.

2.

$$\mu P_1 = \lambda P_0,$$

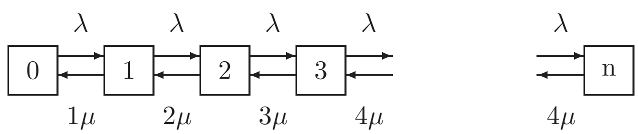


Figure 5.23:

$$\lambda P_0 + 2\mu P_2 = \mu P_1 + \lambda P_1,$$

$$\lambda P_1 + 3\mu P_3 = 2\mu P_2 + \lambda P_2,$$

$$\lambda P_2 + 4\mu P_4 = 3\mu P_3 + \lambda P_3,$$

...

...

...

$$\lambda P_{n-1} + 4\mu P_{n+1} = 4\mu P_n + \lambda P_n,$$

$$\lambda P_n + 4\mu P_{n+2} = 4\mu P_{n+1} + \lambda P_{n+1}.$$

$$P_1 = \frac{\lambda P_0}{\mu},\ P_2 = \frac{(\lambda^2 - \lambda\mu)P_0}{2\mu^2}.$$

$$P_n = \begin{cases} \frac{(\frac{\lambda}{\mu})^n}{n!} P_0, & \text{if } 0 \le n \le 4. \\ \frac{(\frac{\lambda}{\mu})^n}{4!4^{n-4}} P_0, & \text{if } n \ge 4. \end{cases} \tag{5.5}$$

Solve for P_0 and P_n. $s = 4$ in this problem.

$$P_0 = \frac{1}{\sum_{n=0}^{3} \frac{3^n}{n!} + \frac{3^4}{4!} \frac{1}{1-\frac{3}{4}}},\ P_0 = \frac{1}{26.5} = 0.03774.$$

$$P_n = \begin{cases} \frac{3^n}{n!} 0.03774, & \text{if } 0 \le n \le s. \\ \frac{3^n}{4!4^{n-4}} 0.03774, & \text{if } n \ge s. \end{cases} \tag{5.6}$$

3.

$$L_q = \frac{(0.03774)3^4}{4!(1-\frac{3}{4})^2}\left(\frac{3}{4}\right) = \frac{3.05694(3)}{24(\frac{1}{4})^2 4} = \frac{9.17082}{6} = 1.53.$$

$$W_q = \frac{L_q}{\lambda} = \frac{1.53}{3} = 0.51 \text{ mins}, W = W_q + \frac{1}{\mu} = 0.51 + \frac{1}{1} = 1.51 \text{ mins},$$

$$L = L_q + \frac{\lambda}{\mu} = 1.53 + 3 = 4.53.$$

Problem 12: Jobs arrive at a particular work center according to a Poisson input process at a mean rate of two per day, and the operation time has an exponential distribution with a mean of $\frac{1}{4}$ day. Enough in-process storage space is provided at the work center to accommodate three jobs in addition to the one being processed, whereas excess jobs are stored temporarily in a less convenient location. For what proportion of the time will this storage space at the work center be adequate to accommodate all waiting jobs?

Given: $\lambda = \frac{2 \text{ jobs}}{\text{day}}$ and $\mu = 4$. $P(N \leq 4) = P_0 + P_1 + P_2 + P_3 + P_4$. $P_0 = \frac{1}{1+\sum_{n=1}^{\infty}(\frac{1}{2})^n}$. Let $S_n = \frac{1}{2}+\frac{1}{4}+\frac{1}{8}+...+\frac{1}{2^n}$. $2S_n = 1+\frac{1}{2}+\frac{1}{4}+...+\frac{1}{2^{n+1}}$. $2S_n - S_n = -1 + \frac{1}{2^n} - \frac{1}{2-(n+1)} = -1 + \frac{1}{2^n} - \frac{1}{2^{n+1}} = -1 + 2^{-n} - 2^{-(n+1)} = -1 + 2 = 1$. $P_0 = \frac{1}{1+1} = \frac{1}{2}$. $P_n = \rho^n P_0$. $P_1 = \left(\frac{1}{2}\right)^1 \frac{1}{2} = \frac{1}{4}$. $P_2 = \left(\frac{1}{2}\right)^2 \frac{1}{2} = \frac{1}{8}$. $P_3 = \left(\frac{1}{2}\right)^3 \frac{1}{2} = \frac{1}{16}$. $P_4 = \left(\frac{1}{2}\right)^4 \frac{1}{2} = \frac{1}{32}$. $P_0 + P_1 + P_2 + P_3 + P_4 = \frac{1}{2}+\frac{1}{4}+\frac{1}{8}+\frac{1}{16}+\frac{1}{32} = \frac{31}{32}$. $P(N \leq 4) = \frac{31}{32}$.

Problem 17: An airline ticket office has two ticket agents answering incoming phone calls for flight reservations. In addition, one caller can be put on hold until one of the agents is available to take the call. If all three phone lines(both agent lines and the hold line) are busy, a potential customer gets a busy signal, and it is assumed that the call goes to another ticket office and that the business is lost. The calls and attempted calls occur *randomly* (i.e. according to a *Poisson* process) at a mean rate of 15 per hour. The length of a telephone conversation has an *exponential* distribution with a mean of 4 minutes.

1. Construct the rate diagram for this Queuing system.
2. Find the steady state probability that:
   (a) A caller will get to talk to an agent immediately,
   (b) The caller will be put on hold,
   (c) The caller will get a busy signal.

Given: $\lambda = \frac{15 \text{ calls}}{\text{hr}}\frac{1 \text{ hr}}{60 \text{ min}} = \frac{1}{4}$. $\frac{1}{\mu} = 4$ min. Therefore $\mu = \frac{1}{4}$.

1. See Figure 5.24.
2. $P(N \leq 2) = P_0 + P_1 + P_2$, $P_0 = \frac{1}{1+1+\frac{1}{1-2}} = \frac{1}{2.25} = 0.333$. $P_1 = \frac{1}{1}(0.333) = 0.333$, $P_2 = \frac{(1)^2}{2(2)}(0.333) = 0.08325$.
   (a) $P_0 + P_1 = 0.666$.
   (b) $P_3 = \frac{(1)^3}{2!3}(0.333) = 0.056$.
   (c) $P(N \geq 4) = 1 - P(N \leq 4) = 1 - P_0 - P_1 - P_2 - P_3 = 1 - 0.333 - 0.333 - 0.08325 - 0.056 - 0.195$.

Problem 24: Plans are currently being developed for a new factory. One department has been allocated a large number of automatic machines of a certain type, and we need to determine how many machines should be assigned to each operator for servicing(loading,unloading,adjusting, setup, and so on). For the purpose of this analysis, the following information has been provided.

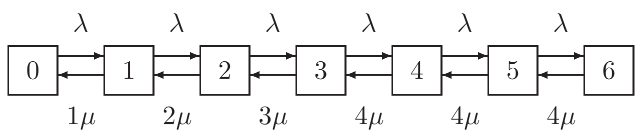


Figure 5.24:

The running time(time between completing service and the machine requiring service again) of each machine has an *exponential* distribution, with a mean of 150 minutes. Each operator attends to her own machine; she does not give help to or receive help from other operators. For the department to achieve the required production rate, the machines must be running at least 89 percent of the time on the average.

1. What is the maximum number of machines that can be assigned to an operator while still achieving the required production rate?
2. Given that the maximum number found in part (a) is assigned to each operator, what is the expected fraction of time that the operators will be busy servicing machines?

It is an M/M/1 model. N is the size of the calling population. $\lambda = \frac{1}{150}, \mu = \frac{1}{15}$.

1. We require that the average number L not working be less than 11% of N. $L < 0.11N$.

$$0.11N > l = N = 10(1 - P_0) = N - 10 + 10P_0,$$

$$10 > 0.89N + 10P_0 = 0.89N + \frac{10}{\sum_{n=0}^{N} \frac{N!}{(N-n)!10^n}} = g(N).$$

   $g(3) = 9.99, g(4) = 10.03$ so no operator can service more than 3 machines.

2. If 3 are assigned, $P_0 = \frac{1}{\sum_{n=0}^{3} \frac{6}{(3-n)!10^n}} = 0.7321$ so the expected time that the operator will be busy is $1 - P_0 = 0.2679$.

Problem 27: Consider the M/G/1 model.

1. Compare the expected waiting time in the queue if the service time distribution is (i) exponential, (ii) constant, (iii) Erlang with the amount of variation (i.e. the standard deviation) halfway between the constant and the exponential cases.
2. What is the effect on the expected waiting time in the queue and on the expected queue length if both λ and μ are doubled and the scale of the service time distribution is changed accordingly?

1. i) M/M/1 $W_q^i = \frac{\lambda}{\mu(\mu-\lambda)}$.

   ii) M/D/1 $W_q^{ii} = \frac{\frac{\lambda}{\mu^2}}{2(1-\frac{\lambda}{\mu})} = \frac{\lambda}{2\mu(\mu-\lambda)} = \frac{1}{2}W_q^i$.

   iii) $M/E_k/1$ $\sigma = \frac{0+\frac{1}{\mu}}{2} = \frac{1}{2\mu}, \sigma^2 = \frac{1}{4\mu^2}$.

$$W_q^{iii} = \frac{1}{\lambda}\left(\frac{\lambda^2\frac{1}{4\mu^2} + \frac{\lambda^2}{\mu^2}}{2(1-\frac{\lambda}{\mu})}\right) = \frac{\frac{5}{4}\frac{\lambda}{\mu^2}}{2(1-\frac{\lambda}{\mu})} = \frac{5}{8}\frac{\lambda}{\mu(\mu-\lambda)} = \frac{5}{8}W_q.$$

2. n denotes quantities for the modified queues created from those in a).

$$\widetilde{W}_q^I = C_j\tilde{W}_q^i = C_j\frac{2\lambda}{2\mu(2\mu-2\lambda)} = \frac{1}{2}C_j\frac{\lambda}{\mu(\mu-\lambda)} = \frac{1}{2}W_q.$$

   Where $C_1 = 1, C_2 = \frac{1}{2}, C_3 = \frac{5}{8}$. Also $\tilde{L}_q^j = 2\lambda\tilde{W}_q^j = 2\lambda\frac{1}{2}W_q = L_q$. Thus, the expected waiting time in the queue is cut in half while expected queue length is unchanged.

Problem 35: Consider the model with *non preemptive priorities* presented in Section 16.8 of the text book. Suppose there are just two priority classes, with $\lambda_1 = 4$ and $\lambda_2 = 4$. In designing this Queuing system, you are offered the choice between the following two alternatives: (1) one fast server (μ =10) and (2) two slow servers ($\mu = 5$).

Compare these alternatives with the usual four mean measures of performance (W, L, W_q, L_q) for the individual priority classes(W_1, W_2, L_1, L_2) and so forth. Which alternative is preferred if your primary concern is expected waiting time in the *system* for priority class 1 (W_1)? Which is preferred if your primary concern is expected waiting time in the *queue* for priority class 1? Alternative 1: $\lambda_1 = 4, \lambda_2 = 4, \mu = 10, s = 1$.

	Priority 1	Priority 2
L	0.9333	3.0667
L_q	0.5333	2.6667
W	0.2333	0.7667
W_q	0.1333	0.6667

Alternative 2: $\lambda_1 = 4, \lambda_2 = 4, \mu = 10, s = 2$.

	Priority 1	Priority 2
L	1.2741	3.1704
L_q	0.4741	2.3704
W	0.3185	0.7926
W_q	0.1185	0.5926

Alternative 1 gives a lower expected system waiting time for priority 1 customers, 0.2333 vs 0.3185 for alternative 2. Alternative 2 gives the lower expected waiting time in the queue for priority 1 customers, 0.1185 vs 0.1333 for alternative 1.

Problem 36: A particular work center in a job shop can be represented as a single server Queuing system, where jobs arrive according to a *Poisson* process, with a mean rate of eight per day. Although the arriving jobs are of three distinct types, the time required to perform any of these jobs has an *exponential* distribution, with a mean of 0.1 working day. The practice has been to work on arriving jobs on a first-come- first-served basis. However, it is important that jobs of type 1 do not have to wait very long, whereas the wait is only moderately important for jobs of type 2 and relatively unimportant for jobs of type 3. These three types arrive with a mean rate of two, four, and two per day, respectively. Because all three types have experienced rather long delays on the average, it has been proposed that the jobs be selected according to an appropriate priority discipline instead.

Compare the expected waiting time(including service) for each of the three types of jobs if the queue discipline is (a) first come first served, (b) non preemptive priority, or (c) preemptive priority.

1. $M/M/1, \lambda = 8, \mu = 10, W = \frac{1}{10-8} = \frac{1}{2}$.
2. $A = \frac{2}{\frac{4}{5}} + 10 = \frac{5}{2} + 10\frac{25}{2}$, $B_0 = 1, B_1 = 1 - \frac{2}{10} = \frac{8}{10}$, $B_2 = 1 - \frac{6}{10} = \frac{4}{10}$, $B_3 = 1 - \frac{8}{10} = \frac{2}{10}$. $\lambda_1 = 2, \lambda_2 = 4, \lambda_3 = 2$.
$$W_1 = \frac{1}{\frac{25}{2}\frac{8}{10}} + \frac{1}{10} = \frac{2}{10} = 0.2,\ W_2 = \frac{1}{\frac{25}{2}\frac{8}{10}\frac{4}{10}} + \frac{1}{10} = \frac{1}{4} + \frac{1}{10} = \frac{7}{10} = 0.35,$$
$$W_3 = \frac{1}{\frac{25}{2}\frac{4}{10}\frac{2}{10}} + \frac{1}{10} = 1 + \frac{1}{10} = 1.1.$$
3. $$W_1 = \frac{\frac{1}{10}}{\frac{8}{10}} = \frac{1}{8} = 0.125,\ W_2 = \frac{\frac{1}{10}}{\frac{8}{10}\frac{4}{10}} = \frac{10}{32} = 0.3125,\ W_3 = \frac{\frac{1}{10}}{\frac{4}{10}\frac{2}{10}} = \frac{10}{8} = 1.25.$$

Problem 38: One inspector has been assigned the full-time task of inspecting the output from a group of 10 identical machines. Jobs to be done by any one of the machines arrive according to a *Poisson* process at a mean rate of 70 per hour. The time required by a machine to perform each job has an *exponential* distribution with a mean of 6 minutes. Thus, whenever all 10 machines are busy, the jobs are being completed ready for inspection at a mean rate of 100 per hour. Unfortunately, the inspector is able to inspect them at a mean rate of only 80 per hour. (In particular, his inspection time has an *Erlang* distribution with a mean of 0.75 minute and a shape parameter $k = 25$). This inspection rate has resulted in a substantial average amount of in-process inventory at the inspection station(i.e. the expected number of jobs waiting to be inspected is fairly large), in addition to that already found at the group of machines. Management feels that there is too much capital tied up in in-process inventory, so it has instructed the production manager to cut down on such inventory. Therefore, the production manager has mad two alternative proposals to reduce the average level of in-process inventory. Proposal 1 is to use slightly less power for the machines(which would increase their expected time to perform a job to 7 minutes), so that the inspector can keep up with their output better. Proposal 2 is to substitute a certain younger inspector for this task. He is somewhat faster(albeit more variable in his inspection times because of less experience), so he should keep up better.(His inspection time would have an *Erlang* distribution with a mean of 0.72 minute and a shape parameter $k = 2$.)

The production manager has asked you to "use the latest OR techniques to see how much each proposal would cut down on in-process inventory"

1. What would be the effect of proposal 1? Why? How would you explain this outcome to the production manager?
2. Determine the effect of proposal 2. How would you explain this outcome to the production manager?
3. What suggestions would you make for reducing the average level of in-process inventory at the inspection station? At the group of machines?

By the Equivalence Property, the input for the inspector is Poisson with $\lambda = 70$ per hour or $\frac{7}{6} = 1.1667$ per minute. The mean inspection time is $\frac{1}{\mu} = \frac{3}{4}$. Since inspection time is Erlang with shape parameter 25 and scale parameter α, $\frac{3}{4} = \frac{1}{\mu} = 25(\frac{1}{\alpha})$. Hence, $\alpha = \frac{100}{3} = 33.3333$. The variance of the service time is $\sigma^2 = 25(\frac{1}{\alpha^2}) = 0.0225$. The model is $M/E_{25}/1$. $L_q = 3.185$.

1. A speed up in the machines or a slow down will not change the steady state output as long as a steady state is reached. Thus proposal 1 has no effect on queue length at the inspection.

2. $M/E_2/1$ model.

3. $M/E_2/1$ $\lambda = 1.1667$ per minute. $\frac{1}{\mu} = 2(\frac{1}{\alpha}) = 0.72$. $\alpha = \frac{1}{0.36} = 2.7778$. $\sigma^2 = 2(\frac{1}{\alpha^2}) = 0.2592$. $L_q = 3.3075$. This is actually a bit worse than the present set up. This results from the higher variance of the new inspector's inspection time.

Problem 45: Consider a system of two *infinite queues in series,* where each of the two service facilities has a single server. All service times are independent and have an exponential distribution, with a mean of 3 minutes at facility 1 and 4 minutes at facility 2. Facility 1 has a Poisson input process with a mean rate of 10 per hour.

1. Find the steady-state distribution of the number of customers at facility 1, and then at facility 2. Then show the *product form solution* for the *joint* distribution of the number at the respective facilities.

2. What is the probability that *both* servers are idle?

3. Find the expected *total* number of customers in the system and the expected *total* waiting time(including service times) for a customer.

1. First facility is M/M/1. $\lambda = 10, \mu = 20, \rho = \frac{1}{2}$. $L_1 = 1, P_{1n} = \frac{1}{2}\frac{1}{2^n}$. The second facility is M/M/1. $\lambda = 10, \mu = 15, \rho = \frac{2}{3}$. $L_2 = 2, P_{2n} = \frac{1}{3}(\frac{2}{3})^n$. $f_{12}(m,n) = P(N_1 = m \text{ and } N_2 = n) = \frac{1}{2}\frac{1}{2^m}\frac{1}{3}(\frac{2}{3})^n = \frac{2^n}{6(2^m)(3^n)}$.

2. $f_{12}(0,0) = \frac{1}{6}$.

3. $L = L_1 + L_2 = 3, W = \frac{L}{\lambda} = \frac{3}{10}$ hrs or 18 minutes.

Problem 46: Under the assumptions specified in Section 16.9 of the text book for a system of *infinite queues in series,* this kind of Queuing network actually is a *special case* of a *Jackson network,* including specifying the values of the a_j and the p_{ij} given λ for this system. See Figure 5.25.

$a_1 = \lambda, a_i = 0$, for $1 \leq i \leq N$ since new customers can only enter at F_1. From each facility a customer always goes to the next. So $p_{ij} = 0$ for $j \neq i+1$, and $p_{ij} = 1$ for $j = i+1, i \neq N$.

Problem 47: Consider a *Jackson network* with three service facilities having the parameter values shown below.

Facility j	s_j	μ_j	a_j	i=1	i=2	i=3
j=1	1	40	10	—	0.3	0.4
j=2	1	50	15	0.5	—	0.5
j=3	1	30	3	0.3	0.2	—

1. Find the *total* arrival rate at each of the facilities.

2. Find the steady-state distribution of the number of customers at facility 1. At facility 2. At facility 3. Then show the *product form solution* for the *joint* distribution of the number at the respective facilities.

3. What is the probability that *all* the facilities have *empty queues* (no customers waiting to begin service)?

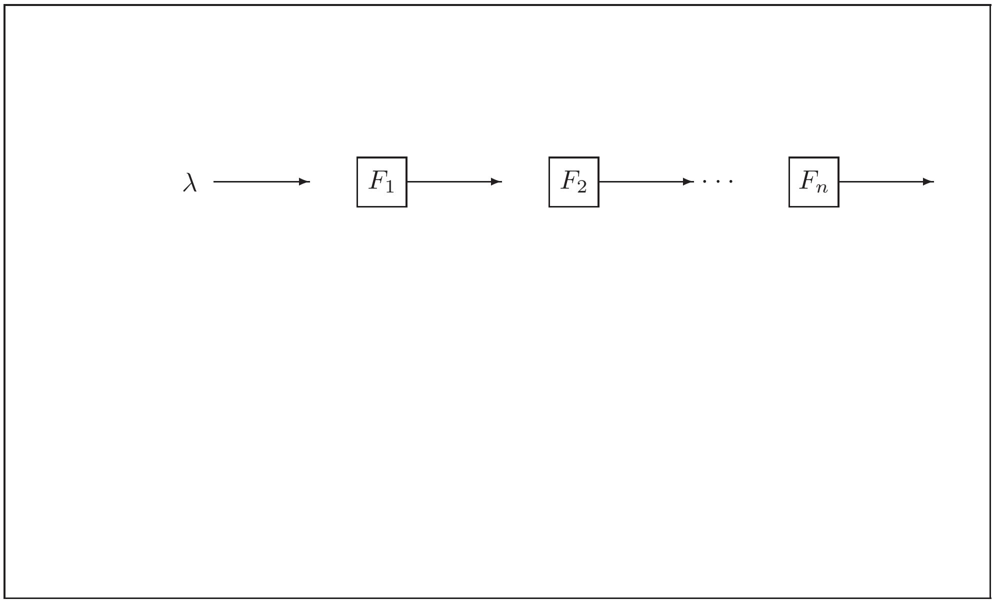


Figure 5.25:

4. Find the expected *total* number of customers in the system.

5. Find the expected *total* waiting time (including service times) for a customer.

See Figure 5.26.

1. $\lambda_1 = 10 + 0.3\lambda_2 + 0.4\lambda_3,\ \lambda_2 = 15 + 0.5\lambda_1 + 0.5\lambda_3,\ \lambda_3 = 3 + 0.3\lambda_1 + 0.2\lambda_2,$ Therfore, $\lambda_1 = 30, \lambda_2 = 40, \lambda_3 = 20$.

2. For $F_1 : \lambda_1 = 30, \mu_1 = 40, \rho_1 = \frac{3}{4}, L_1 = 3$. For $F_2 : \lambda_2 = 40, \mu_2 = 50, \rho_2 = \frac{4}{5}, L_2 = 4$. For $F_3 : \lambda_3 = 20, \mu_3 = 30, \rho_3 = \frac{2}{3}, L_3 = 2$.

$$P(N_1 = n_1, N_2 = n_2, N_3 = n_3) = \frac{1}{4}\left(\frac{3}{4}\right)^{n_1}\frac{1}{5}\left(\frac{4}{5}\right)^{n_2}\frac{1}{3}\left(\frac{2}{3}\right)^{n_3}.$$

3. $P(N_1 = 0, N_2 = 0, N_3 - 0) = (\frac{1}{4})(\frac{1}{5})(\frac{1}{3}) = \frac{1}{60}$.

4. $L = L_1 + L_2 + L_3 = 3 + 4 + 2 = 9$.

5. $W = \frac{L}{\lambda}$. $\lambda = a_1 + a_2 + a_3 = 10 + 15 + 3 = 28$. $W = \frac{9}{28}$.

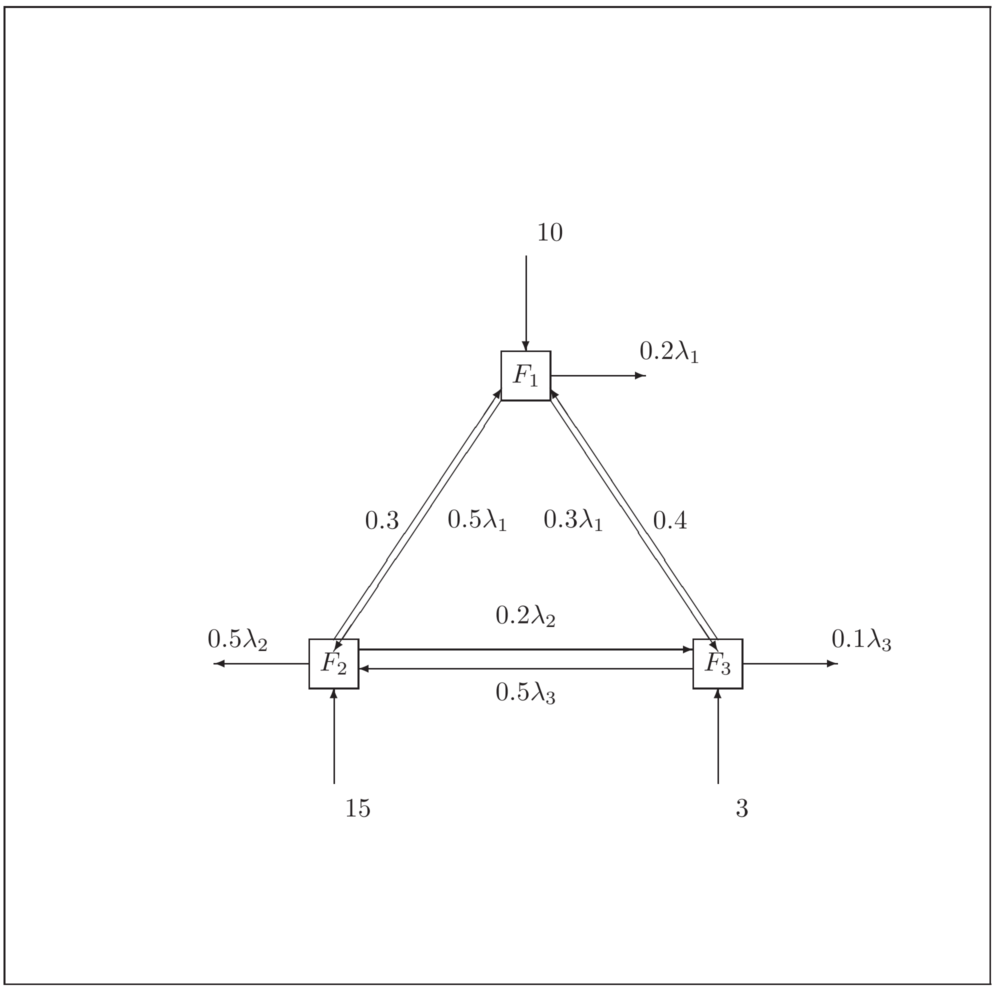

10
F_1
$0.2\lambda_1$
0.3
$0.5\lambda_1$
$0.3\lambda_1$
0.4
$0.5\lambda_2$
F_2
$0.2\lambda_2$
F_3
$0.1\lambda_3$
$0.5\lambda_3$
15
3

Figure 5.26:

5.3.8 Handout of Equations

	$M/M/1/\infty$	$M/M/s/\infty$	$M/M/1/k$	$M/M/s/s$
P_0	$1-\rho$	$\frac{1}{\sum_{n=0}^{s-1}\frac{(\frac{\lambda}{\mu})^n}{n!}+\frac{(\frac{\lambda}{\mu})^s}{s!}\frac{1}{1-\frac{\lambda}{s\mu}}}$	$\frac{1-\rho}{1-\rho^{k+1}}$	$\frac{1}{1+\sum_{n=1}^{s}\frac{(\frac{\lambda}{\mu})^n}{n!}+\frac{(\frac{\lambda}{\mu})^s}{s!}\sum_{n=s+1}^{k}(\frac{\lambda}{s\mu})^{n-s}}$
P_n	$(1-\rho)\rho^n$	$\frac{(\frac{\lambda}{\mu})^n}{n!}P_0$, if $0\leq n\leq s$. $\frac{(\frac{\lambda}{\mu})^n}{s!s^{n-s}}P_0$, if $n\geq s$.	$\rho^n P_0$	$\frac{(\frac{\lambda}{\mu})^n}{n!}P_0$, for $n=1,2,...,s$. $\frac{(\frac{\lambda}{\mu})^n}{s!s^{n-s}}P_0$, for $n=s,s+1,...,k$.
L	$\frac{\lambda}{\mu-\lambda}$	$L_q+\frac{\lambda}{\mu}$	$\frac{\rho}{1-\rho}-\frac{(k+1)\rho^{k+1}}{1-\rho^{k+1}}$	$\sum_{n=0}^{s-1}nP_n+L_q+s\left(1-\sum_{n=0}^{s-1}P_n\right)$
L_q	$\frac{\lambda^2}{\mu(\mu-\lambda)}$	$\frac{P_0(\frac{\lambda}{\mu})^s\rho}{s!(1-\rho)^2}$	$L-(1-P_0)$	$\frac{P_0(\frac{\lambda}{\mu})^s\rho}{s!(1-\rho)^2}[1-\rho^{k-s}-(k-s)\rho^{k-s}(1-\rho)]$
W	$\frac{1}{\mu-\lambda}$	$\frac{L}{\lambda}$	$\frac{L}{\lambda(1-P_k)}$	$\frac{L}{\lambda(1-P_k)}$
W_q	$\frac{\lambda}{\mu(\mu-\lambda)}$	$\frac{L_q}{\lambda}$	$\frac{L_q}{\lambda(1-P_k)}$	$\frac{L_q}{\lambda(1-P_k)}$
ρ	$\frac{\lambda}{\mu}$	$\frac{\lambda}{s\mu}$	$\frac{\lambda}{\mu}$	$\frac{\lambda}{s\mu}$

For $M/M/1/\infty: P(W>t)=e^{-\mu(1-\rho)t}$ for $t\geq 0$. $M/M/s/\infty: P(W>t)=e^{-\mu t}\left[1+\frac{P_0(\frac{\lambda}{\mu})^s}{s!(1-\rho)}\left(\frac{1-e^{-\mu k(s-1\frac{\lambda}{\mu})}}{s-1-\frac{\lambda}{\mu}}\right)\right]$. $M/G/1/\infty$: Let service time have mean $\frac{1}{\mu}$ and variance ψ^2. $\rho=\frac{\lambda}{\mu}$, $P_0=1-\rho$, $L_q=\frac{\lambda^2\psi^2+\rho 2}{2(1-\rho)}$, $L=\rho+L_q$, $W_q=\frac{L_q}{\lambda}$, $W=W_q+\frac{1}{\mu}$. Finite calling population: Let n be the size of the calling population.

	M/M/1	M/M/s
P_0	$\frac{1}{\sum_{n=0}^{M}\frac{M!}{(M-n)!}(\frac{\lambda}{\mu})^n}$	$\frac{1}{\sum_{n=0}^{s-1}\frac{M!}{(M-n)!n!}(\frac{\lambda}{\mu})^n+\sum_{n=s}^{M}\frac{M!}{(M-n)!s!s^{n-s}}(\frac{\lambda}{\mu})^n}$
P_n	$\frac{M!}{(M-n)!}(\frac{\lambda}{\mu})^n P_0$	$P_0\frac{M!}{(M-n)!n!}(\frac{\lambda}{\mu})^n$, for $0\leq n\leq s$. $P_0\frac{M!}{(M-n)!s!s^{n-2}}(\frac{\lambda}{\mu})^n$, for $s\leq n\leq M$.
L_q	$M-\frac{\lambda+\mu}{\lambda}(1-P_0)$	
L	$M-\frac{\mu}{\lambda}(1-P_0)$	
$W-q$	$\frac{M}{\lambda(M-L)}-\frac{\lambda+\mu}{\lambda^2(n-2)}(1-P_0)$	
W	$\frac{L}{\lambda(M-L)}$	

5.3.9 Summary

- $N(t)$ is a random variable for each $t > 0$.
- Assumptions:
  1. $N(0) = 0$.
  2. $N(t+s) - N(s)$ has a Poisson distribution with mean $\lambda\pi$. λ is the mean rate per unit of time. Therefore, $P[N(t+s) - N(s) = n] = \frac{e^{-\lambda t}(\lambda t)^n}{n!}$, for $n = 0, 1, 2, 3, ...$
  3. If $0 \le t_1 \le t_2 \le t_3 \le ... \le t_n$ then $N(t_1) - N(0), N(t_2) - N(t_1), N(t_3) - N(t_2), ...$ are independent random variables. Therefore, given 1,2,3 N(t) is a *Poisson process.*
- T is the time until the first observation. $P(T \le t) = 1 - e^{-\lambda t}$.
- The *memoryless property:* $P(T > t - s | T > s) = e^{-\lambda t} = P(T > t)$.
- The time between two events in a Poisson process has an *exponential density* $\lambda e^{-\lambda t}$. Therefore, $P(T \le t) = e^{-\lambda t}$.
- $E(T_i) = \frac{1}{\alpha_i}$. Let $m = \min(T_1, T_2, ..., T_i), 1 \le i \le m$. m has an exponential density with mean

  $$\frac{1}{\sum_{i=1}^{m} \alpha_i}.$$

- $\upsilon_n = \sum_{i=1}^{n} T_i$. Each T_i is an exponential distribution with mean $\frac{1}{\lambda}$.

  $$P(\upsilon_n \le t) = 1 - \sum_{i=0}^{n-1} \frac{e^{-\lambda t}(\lambda t)^i}{i!}.$$

  The *Erlang density* if $f_{\upsilon_n}(t) = \lambda e^{-\lambda t} \frac{\lambda^n t^{n-1}}{(n-1)!}, 0 \ge t$. It is also a *gamma density.*
- $E(\upsilon_n) = \sum_{i=1}^{n} E(T_i) = \sum_{i=1}^{n} \frac{1}{\lambda_i}$. In general, $\frac{n}{\lambda}$.
- $\sigma^2_{\upsilon_n} = \sum_{i=1}^{n} \sigma^2_{T_i} = \frac{n}{\lambda^2}$.
- Queue notation(type of model):

  arrival distribution/service time distribution/number of servers/system capacity/ calling population/service discipline.

  Or,

  /arrival distribution/service time distribution/$s/k/N/$service discipline.
- The *steady state equations* are derived from the rate-in = rate-out principle. The following derivations are based on the Geometric series. $m/m/1 : C_n = \frac{\lambda_{n-1}\lambda_{n-2}...\lambda_0}{\mu_n\mu_{n-1}...\mu_1}$, for $n = 1, 2, 3, ...$

  The following equations are $\sim$ *exponential*$(\mu(1-\rho))$

  $P_n = C_n P_0$, $P_0 = \frac{1}{1+\sum_{n=1}^{\infty} C_n}$, $L = \sum_{n=0}^{\infty} nP_n$ $L_q = \sum_{n=s}^{\infty}(n-s)P_n$ $W = \frac{L}{\lambda}$ $W_q = \frac{L_q}{\lambda}$ $\bar{\lambda} = \sum_{n=0}^{\infty} \lambda_n P_n$. $P(W > t) = e^{-\mu(1-\rho)t}$ $P(W_q > t) = \rho e^{-\mu(1-\rho)t}$

5.4 Applications of Queuing Theory

- $E(W_c) = \sum_{n=0}^{\infty} g(n)P_n$ for the discrete cases, or $E(g(n))$ for the continuous cases when $g(n)$ is linear, $g(n) = C_w N$ and $E(W_c) = C_w \sum_{n=0}^{\infty} nP_n = C_w L$.
- $E(h(W)) = \int_0^{\infty} h(w) f_W(w)\, dw$, where $f_W(w)$ is the pdf. $E(W_c) = \lambda E(h(W))$.
- For an unknown s, minimize $E(T_c) = sC_s + E(W_c)$ for certain values of s.
- For an unknown μ and s, given λ, and $f(\mu)$, $E(T_c) = sf(\mu) + E(W_c)$.
- For an unknown λ and s given μ, C_s, C_f, and λ_ρ,

  $$E(T_c) = n[(C_f = sC_s) + E(W_c) + \lambda C_t E(T)],$$

  where C_t is the expected travel cost.
- Evaluation of travel time with uniform x, y(customers),

  $$E(T) = \frac{2}{v}(E(|x|) + E(|y|),\ E(|x|) = \frac{a^2 + c^2}{2(a+c)},\ E(|y|) = \frac{b^2 + d^2}{2(b+d)},$$

  or with pdf's(marginal) use,

  $$E(|x|) = \int_{-\infty}^{\infty} x f_{|x|}(x)\, dx,\ E(|y|) = \int_{-\infty}^{\infty} y f_{|y|}(y)\, dy.$$

5.4.1 M/M/1 Taxi Example

Taxi's arrive at random 1 every 2 minutes and customers arrive at random 1 every 3 minutes. Taxi's do not wait if no one is there. What fraction of the cabs leave the stand empty? What is the expected waiting time for a customer? It is given that the customers are passengers and arrive as a Poisson process with mean $\lambda = \frac{1}{3}$. This is an M/M/1 model. See Figure 5.27.

Service consists of being next in line and service is exponential with a mean of 2. So, $\frac{1}{\mu} = 2$, or $\mu = \frac{1}{2}$. $\rho = \frac{\lambda}{\mu}$. To answer the first question, P(N=0) $= P_0 = 1 - \rho = 1 - \frac{2}{3} = \frac{1}{3}$. To answer the second question, $W = \frac{1}{\frac{1}{2} - \frac{1}{3}} = 6min$. This includes the taxi ride time, also. What is the expected number of people at the stand? $L = \lambda W = \left(\frac{1}{3}\right) 6 = 2$. $P(W > t) = e^{-\mu(1-\rho)t}$, $f_W(t) = \mu(1-\rho)e^{-\mu(1-\rho)t}, t > 0$, $f_W(t) = \frac{1}{2}\frac{1}{3}e^{-\frac{1}{2}\frac{1}{3}t} = \frac{1}{6}e^{-\frac{1}{6}t}$, $P(W > 3) = \int_3^{\infty} f_W(t)\, dt = \int_3^{\infty} \frac{1}{6}e^{-\frac{1}{2}t}\, dt = e^{-\frac{1}{6}t}\Big|_3^{\infty} = -0 - (-e^{-\frac{1}{2}}) = e^{-\frac{1}{2}} = 0.606$. W_q is the waiting time in queue. $W_q = E(W_q)$. $P(W_q > t), t > 0$. $P(W_q > t) = \sum_{n=1}^{\infty} P_n P(S_n > t) = \sum_{n=1}^{\infty}(1-\rho)\rho^n \int_t^{\infty} \frac{\mu^n z^{n-1}}{(n-1)!}e^{-\mu z}\, dz = \mu(1-\rho)\rho \int_t^{\infty} e^{-\mu z} \sum_{n=1}^{\infty} \frac{(\mu\rho z)^{n-1}}{(n-1)!}\, dz = \mu(1-\rho)\rho \int_t^{\infty} e^{-\mu z} e^{\mu\rho z}\, dz = \mu(1-\rho)\rho \int_t^{\infty} e^{-\mu(1-\rho)z}\, dz = \frac{\mu(1-\rho)\rho e^{-\mu(1-\rho)z}}{-\mu(1-\rho)}\Big|_t^{\infty} = -P(0 - e^{-\mu(1-\rho)t})$. Therefore, $P(W_q > t) = \rho e^{-\mu(1-\rho)t}$.

5.4.2 The Berth Example

A company owns a berth at a port. Ships arrive for unloading on an average of 1 every 12 hours as a Poisson process. Unloading times are exponential with mean n hours. Running costs for the berth are $\frac{\$20{,}000}{n}$ per day plus \$2,000 per ship day delay at anchorage. Find the value of n that minimizes total costs.

Let T be the total cost per day. $T = \frac{20{,}000}{n} + 2{,}000 N_q$. $E(T) = \frac{20000}{n} + 2000 L_q = \frac{20000}{n} + \frac{2000\lambda^2}{\mu(\mu-\lambda)}$. $\lambda = 2, \mu = \frac{24}{n}$. Therefore, $E(T) = \frac{20000}{n} + \frac{2000(4)}{\frac{24}{n}(\frac{24}{n} - 2)} = \frac{20000}{n} + \left(\frac{8000}{24}\right)\left(\frac{n^2}{24 - 2n}\right) = \frac{20000}{n} + \frac{4000n^2}{24(12-n)}$, with the restriction that $0 < n < 12$. Alternatively, use differentiation, $n = 6.135$ or $n = 22.8179$. n must be 6.135 due to the restriction on n.

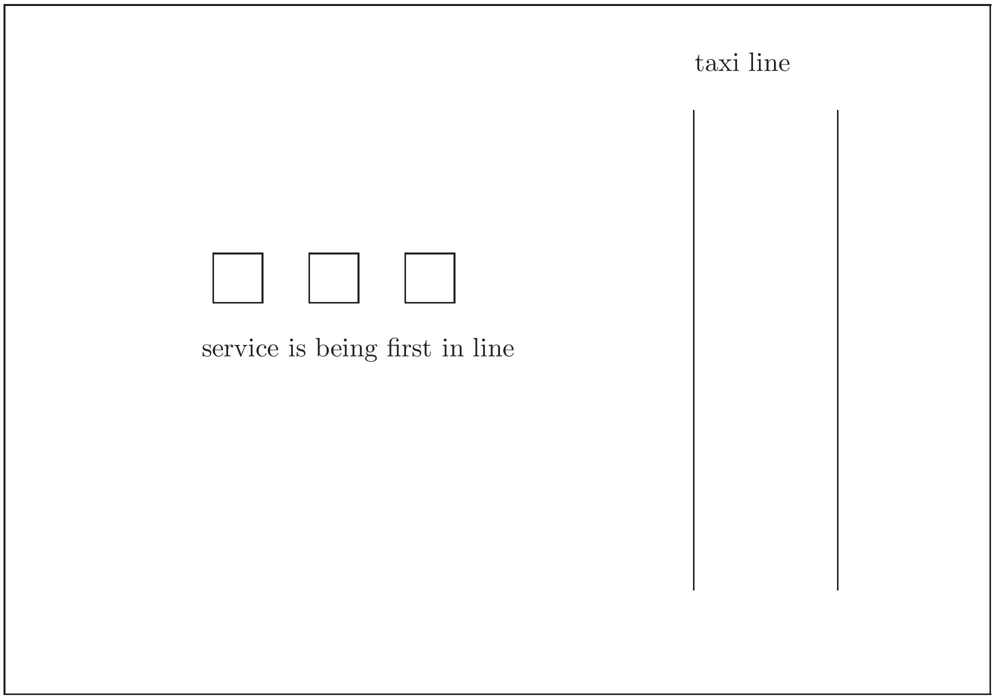


Figure 5.27:

5.4.3 Homework and Answers

Do problems 5, 8, 13, 23 in the text book.

Problem 5: The problem is to choose between two types of materials-handling equipment, A and B, for transporting certain types of goods between certain producing centers in a job shop. Calls for materials-handling unit to move a load would come essentially at random(i.e. according to a *Poisson* input process) at a mean rate of four per hour. The total time required to move a load has an *exponential* distribution, where the expected time is 12 minutes for A and 9 minutes for B. The total equivalent uniform hourly cost(capital recovery cost plus operating cost) would be \$50 for A and \$150 for B. The estimated cost of idle goods (waiting to be moved or in transit) because of increased in-process inventory is \$20/load/hour. Furthermore, the scheduling of the work at the producing centers allows for just 1 hour from the completion of a load at one center to the arrival of that load at the next center. Therefore, an additional \$100/load/hour of delay(including transit time) *after the first hour* is to be charged for lost production because of idle personnel and equipment, extra costs of expediting and supervision, and so forth.

Assuming that only one materials-handling unit is to purchased, which type of unit should be selected? This is an M/M/1 model, $\lambda = 4, \mu_A = 5, \mu_B = \frac{20}{3}$.

$$E(WC) = \lambda \left(\int_0^1 20t(\mu-\lambda)e^{-(\mu-\lambda)t}\, dt + \int_1^\infty [20 + 100(t-1)](\mu-\lambda)e^{-(\mu-\lambda)}\, dt \right) =$$

$$20\lambda(-te^{-(\mu-\lambda)t})\Big|_0^1 + \int_0^1 e^{-(\mu-\lambda)t}\, dt + e^{-(\mu-\lambda)} + 5\int_0^\infty z(\mu-\lambda)e^{-(\mu-\lambda)t}\, dt ... =$$

$$20\lambda(-e^{-(\mu-\lambda)}) - \frac{e^{-(\mu-\lambda)t}}{\mu-\lambda}\Big|_0^1 + \left(e^{-(\mu-\lambda)} + \frac{5e^{-(\mu-\lambda)}}{\mu-\lambda}\right) = \frac{20\lambda}{\mu-\lambda}\left(1 + 4e^{-(\mu-\lambda)}\right) =$$

$$\begin{cases} 80\left[1+\frac{4}{e}\right] = 197.72, & \text{for A} \\ 4\frac{15}{2}\left[1+\frac{4}{e^{\frac{8}{3}}}\right] = 38.34, & \text{for B} \end{cases}$$

$$E(TC) = E(SC) + E(WC)\begin{cases} 50 + 197.72, & \text{for A} \\ 150 + 38.34, & \text{for B} \end{cases}$$

Therefore, purchase type B.

Problem 8: A particular in-process inspection station is used to inspect sub assemblies of a certain kind. At present there are two inspectors at the station, and they work together to inspect each subassembly. The inspection time has an *exponential* distribution, with a mean of 15 minutes. The cost of providing this inspection system is \$20/hour.

A proposal bas been made to streamline the inspection procedure so that is can be handled by only one inspector. This inspector would begin by visually inspecting the exterior of the subassembly, and he would then use new efficient equipment to complete the inspection. The times required for these two phases of the inspection have independent *Erlang* distributions, with shape parameter $k = 2$ and means of 6 and 12 minutes, respectively. The capitalized cost of providing this inspection system would be \$15/hour.

The sub assemblies arrive at the inspection station according to a Poisson process at a mean rate of three per hour. The cost of having the sub assemblies wait at the inspection station(thereby increasing in-process inventory and disrupting subsequent production) is estimated to be \$10/hour for each subassembly.

Determine whether to continue the status quo or adopt the proposal in order to minimize expected total cost per hour. $\lambda = 3$. In the status quo, we have M/M/1 with $\mu = 4$. $E(TC) = E(SC) + E(WC) = 20 + 10l = 20+10(3) = 50 >$ In the proposed scheme, we have a general service with mean $\frac{1}{\mu} = \frac{1}{10}+\frac{1}{5} = \frac{3}{10}$ in hours and $\sigma^2 = \frac{2}{400} + \frac{2}{100} = \frac{1}{40}$. $E(TC) = E(SC) + E(WC) = 15 + 10L = 15 + 10(\frac{9}{10} + \frac{\frac{9}{40}+\frac{81}{100}}{\frac{1}{5}}) = 15 + 10(\frac{9}{10} + \frac{207}{40}) = 75.75$. Select the status quo.

Problem 13: A machine shop contains a grinder for sharpening the machine cutting tools. A decision must now be made on the speed at which to set the grinder. The grinding time required by a machine operator to sharpen his cutting tool has an *exponential* distribution, where the mean $\frac{1}{\mu}$ can be set at anything from $\frac{1}{2}$ minute to 2 minutes, depending upon the speed of the grinder. The running and maintenance costs go up rapidly with the speed of the grinder, so the estimated cost per minute for providing a mean of $\frac{1}{\mu}$ is \$ $(0.10\mu^2)$.

The machine operators arrive to sharpen their tools according to a *Poisson* process at a mean rate of one every 2 minutes. The estimated cost of an operator being away from his machine to the grinder is \$0.20/minute.

Plot the expected total cost per minute E(TC) versus μ over the feasible range for μ to solve graphically for the minimizing value of μ. We have an M/M/1 queue with $\lambda = \frac{1}{0.2}$, $\frac{1}{2} < \mu \leq 2$. $E(TC) = E(SC)+E(WC) = 0.1\mu^2 + 0.2L = 0.1\mu^2 + \frac{0.1}{\mu-\frac{1}{2}} = 0.1(\mu^2 + \frac{1}{\mu-\frac{1}{2}})$.

μ	E(TC)
1	0.3
1.1	0.2877
1.15	0.286096
1.155	0.286074
1.16	0.286075
1.17	0.286144

Choose $\mu = 1.155$ since it has the lowest expected total cost.

Problem: 23: A certain job shop has been experiencing long delays in jobs through the turret lathe department because of inadequate capacity. The foreman contends that five machines are required, as opposed to the three machines that he now has. However, because of pressure from management to hold down capital expenditures, only one additional machine will be authorized unless there is solid evidence that a second one is necessary.

This shop does three kinds of jobs, namely, government jobs, commercial jobs, and standard products. Whenever a turret lathe finishes a job, it starts a government job if one is waiting; if not, it starts a commercial job if any are waiting; if not, it starts on a standard product if any are waiting. Jobs of the same type are taken on a first-come-first-served basis.

Although much overtime work is required currently, management wants the turret lathe department to operate on an 8 hour, 5 day a week basis. The probability distribution of the time required by a turret lathe for a job appears to be approximately *exponential,* with a mean of 10 hours. Jobs come into the shop according to a *Poisson* input process, but at a mean rate of 6 per week for government jobs, 4 per week for commercial jobs, and 2 per week for standard products.(These figures are expected to remain the same for the indefinite future.)

It is worth about \$750, \$450, and \$150 to avoid a delay of one additional (working) day in a government, commercial, and standard job, respectively. The incremental capitalized cost of providing each turret lathe(including the operator and so on) is estimated to be \$250/working day.

Determine the number of *additional* turret lathes that should be obtained to minimize expected total cost. This is an M/M/s non-preemptive priority queue model. $\mu = 4, \lambda_1 = 6, \lambda_2 = 4, \lambda_3 = 2, \lambda = 12, \rho = 3, s = 4.$

$$A_4 = 24\left(\frac{16-12}{81}\right)\left[1+3+\frac{9}{2}+\frac{9}{2}\right]+16 = 31.41.$$

$$B_1 = 1-\frac{6}{16} = \frac{5}{8},\ B_2 = 1-\frac{10}{16} = \frac{3}{8},\ B_3 = 1-\frac{12}{16} = \frac{1}{4}.$$

$$W_1 = \frac{8}{(31.41)5}+\frac{1}{4},\ W_2 = \frac{64}{(31.41)15}+\frac{1}{4},\ W_3 = \frac{34}{(31.41)3}+\frac{1}{4}.$$

$$L_1 = 6W_1 = 1.8057,\ L_2 = 4W_2 = 1.5434,\ L_3 = 2W_3 = 1.1792.$$

$$E(TC) = E(SC)+E(WC) = 5000+5[750L_1+450L_2+150L_3] = 16128.4.$$

With $s = 5$,

$$A_5 = 120\left(\frac{16-12}{243}\right)\left[1+3+\frac{9}{2}+\frac{9}{2}+\frac{81}{24}\right]+200 = 52.35.$$

$$B_1 = 1-\frac{6}{20} = \frac{7}{10},\ B_2 = 1-\frac{10}{20} = \frac{1}{2},\ B_3 = 1-\frac{12}{20} = \frac{2}{5}.$$

$$L_1 = 6W_1 = 6\left[\frac{10}{A_5 7}+\frac{1}{4}\right] = 1.6637,\ L_2 = 4W_2 = 4\left[\frac{20}{A_5 7}+\frac{1}{4}\right] = 1.2183,$$

$$L_3 = 2W_3 = 2\left[\frac{5}{A_5}+\frac{1}{4}\right] = 0.6910.$$

$$E(TC) = E(SC)+E(WC) = 6250+5[750L_1+450L_2+150L_3] = 15748.39.$$

Buy two more lathes.

5.5 Inventory Theory

5.5.1 Deterministic Inventory Theory

- k is the setup costs or ordering cost.
- c is the cost per item.
- h is the holding cost per item per time period held.
- p is the shortage cost per item per time period item is out of stock.
- a is the rate at which items are demanded or taken from inventory.
- Q is the order size.

$\frac{Q}{a}$ is called the *cycle length.* See Figure 5.28.

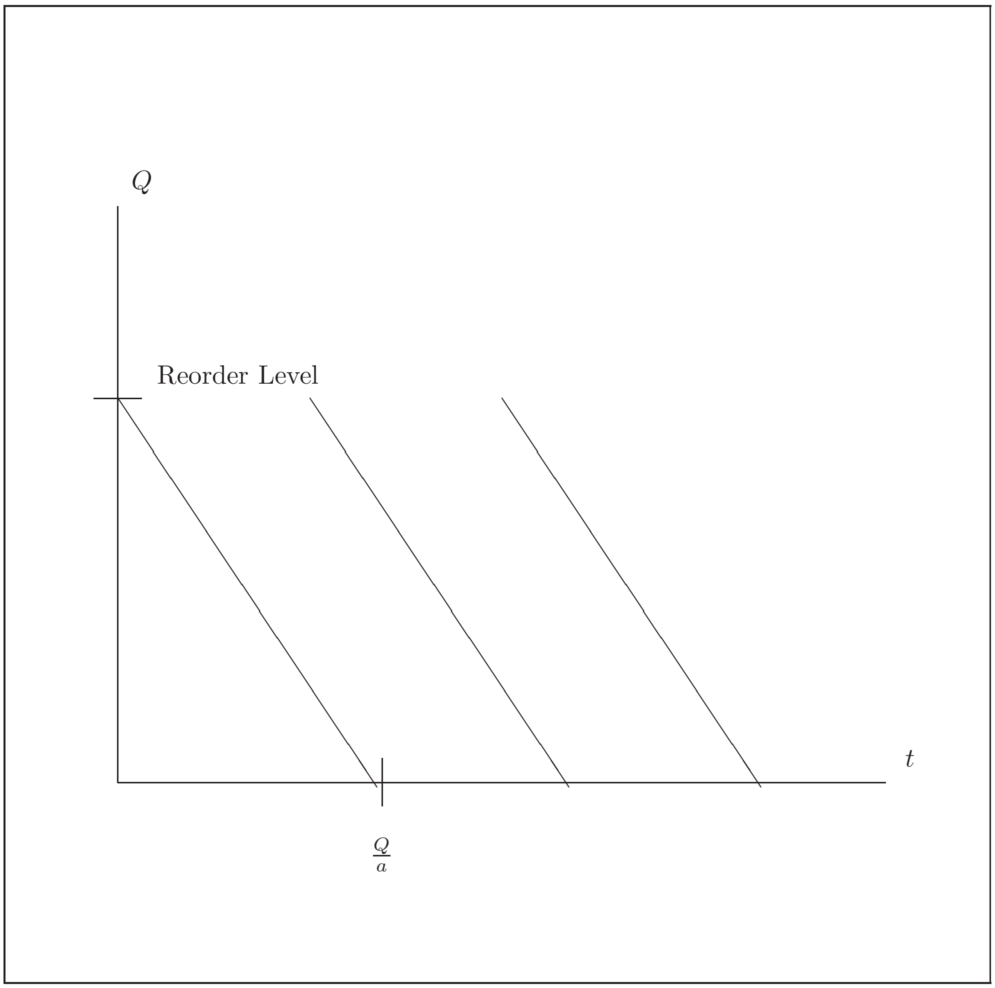


Figure 5.28:

The holding cost is given by the following equation:

$$\sum_{i=1}^{n} hI(t_i)(t_i - t_{i-1}) = \int_a^b hI(t)\,dt.$$

See Figure 5.29.

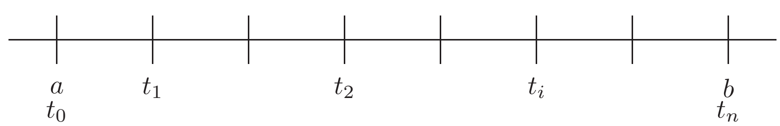


Figure 5.29:

$I(t) = Q - at$, $0 \le t \le \frac{Q}{a}$. The holding cost for one cycle is

$$\int_0^{\frac{Q}{a}} h(Q-at)\,dt = h\int_0^{\frac{Q}{a}} Q - at\,dt = h\frac{(Q-at)^2}{-2a}\bigg|_0^{\frac{Q}{a}} = 0 + \frac{hQ^2}{2a}.$$

Let m be the total holding cost per cycle. Then m is $k + cQ + \frac{hQ^2}{2a}$, not allowing for shortages. We want to minimize the cost per unit of time. Let T be the cost per unit of time. Then, $T = \frac{m}{\frac{Q}{a}} = \frac{ka}{Q} + ca + \frac{hQ}{2}, 0 < Q$. $\frac{dt}{dq} = \frac{-ka}{Q^2} + \frac{h}{2} = \frac{h}{2Q^2}\left(Q^2 - \frac{2ka}{h}\right)$. Therefore, the size of the order should be, $Q = \sqrt{\frac{2ka}{h}}$. The optimum cycle length is $\frac{Q}{a} = \sqrt{\frac{2k}{ha}}$.

Example: A manufacturer of industrial bearings produces bearings of a certain type on an automobile machine at a rate of R per day. Demand for bearings is a per day where $R > a$. At the beginning of each cycle, the machine is started and produces Q bearings. There are startup costs of k each time the machine starts up. There is a production cost of c per item. The cost of items in inventory to be stored is h per bearing per day. Shortages are allowed, but result in back orders and a shortage cost of b per item per day is incurred. Let V be the shortage at the beginning of each cycle. See Figure 5.30 and Figure 5.31.

$$I(t) = \begin{cases} (R-a)t - V, & \text{for } 0 \le t \le \frac{Q}{R} \\ Q - V - at, & \text{for } \frac{Q}{R} \le t \le \frac{Q}{a} \end{cases} \tag{5.7}$$

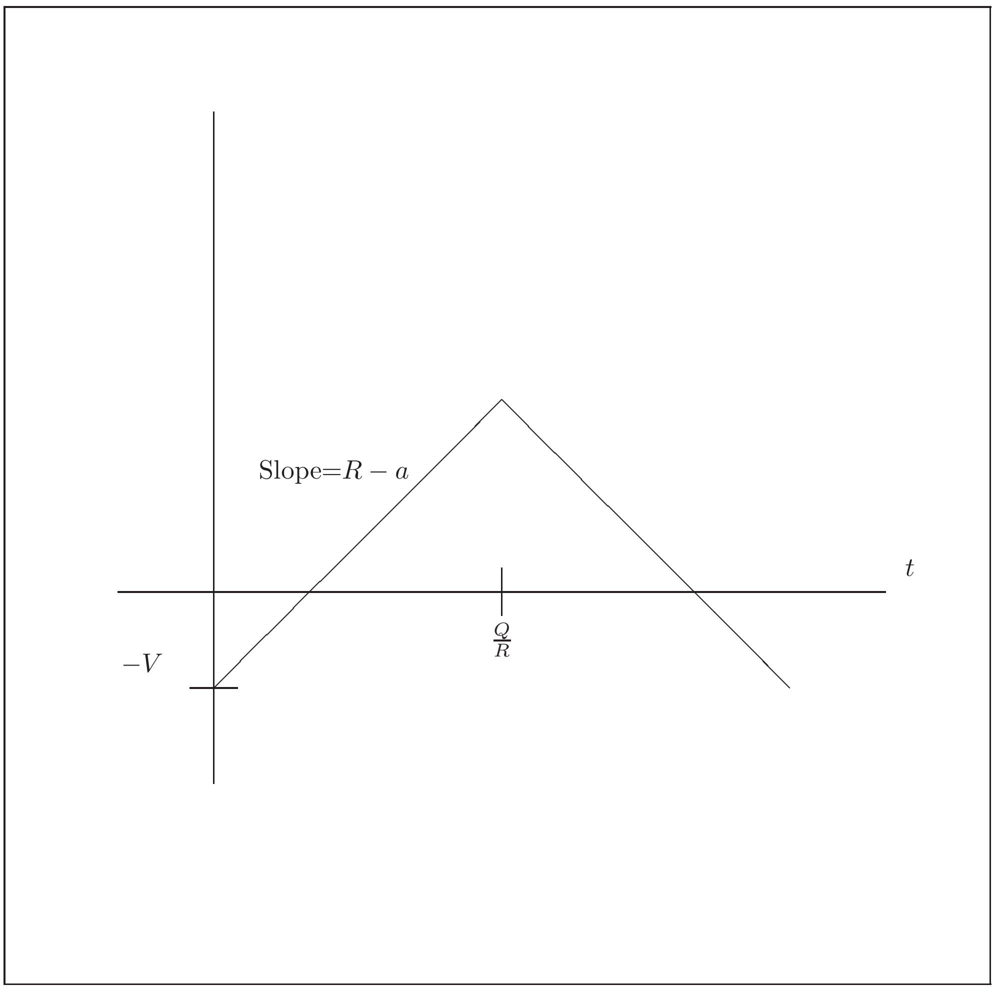


Figure 5.30:

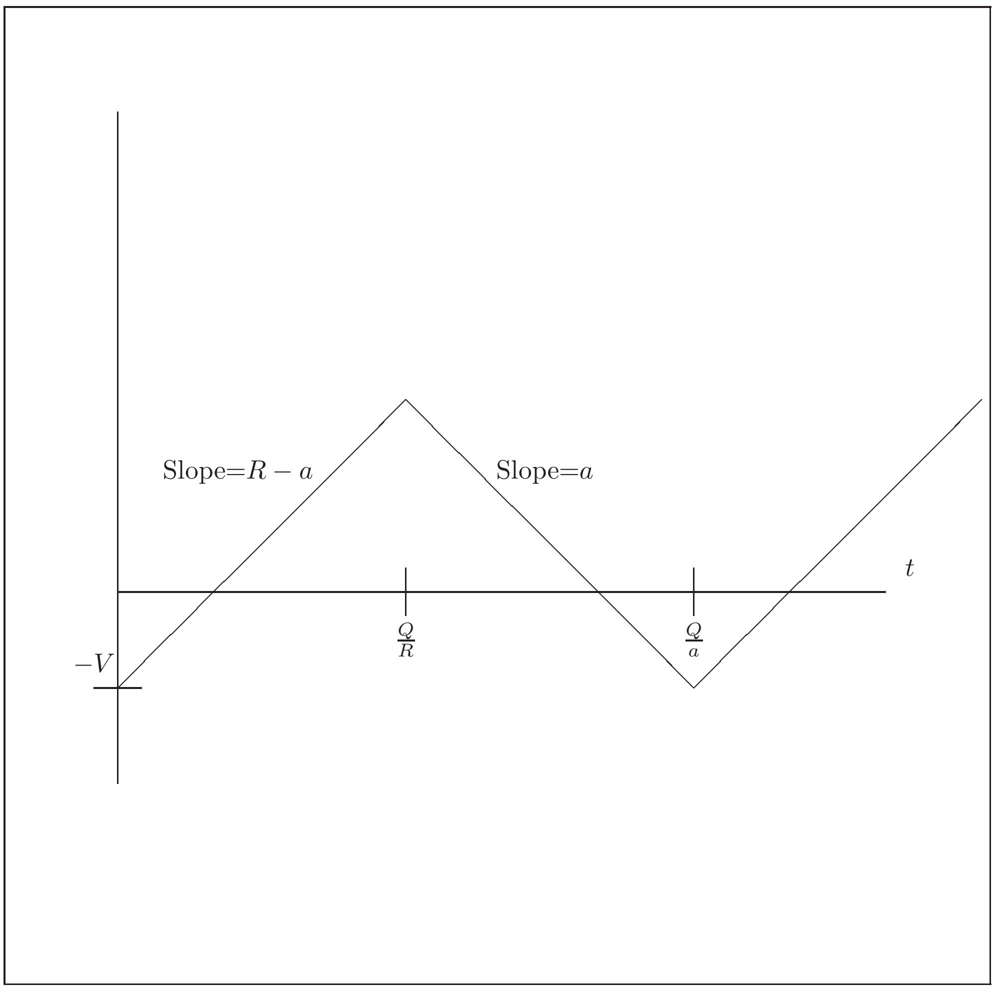


Figure 5.31:

The holding cost per cycle is given by,

$$h\int_{\frac{V}{k-a}}^{\frac{Q-V}{a}} I(t)\,dt =$$

$$h\frac{1}{2}\left[(R-a)\left(\frac{Q}{R}\right)-V\right]\left(\frac{Q-V}{a}-\frac{V}{R-a}\right)=\frac{h}{2aR(R-a)}[(R-a)Q-VR]^2.$$

5.5.2 Probabilistic Inventory Theory

- c is the cost per item.
- h is the holding cost per item.
- ρ is the shortage cost.
- D is random demand.
- ϕ is the density of D.
- Φ is the distribution of D.
- x is the inventory before ordering.
- $M(y)$ is the expected cost if the amount $y-x$ is ordered.

$$M(y) = C(y-x) + h\int_0^y (y-z)\Phi(z)\,dz + \rho\int_y^\infty (z-y)\Phi(z)\,dz.$$

$$\frac{dM(y)}{dy} = c + h\left[(Y-y)\phi(y)(1) + \int_0^y \phi(z)\,dz] + \rho[(Y-y)\phi(y) + \int_y^\infty -\phi(z)\,dz\right] =$$

$$c + h\int_0^y \phi(z)\,dz - \rho\int_y^\infty \phi(z)\,dz = c + h\Phi(y) - \rho[1-\Phi(y)] = c - \rho + (h+\rho)\Phi(y).$$

Set the above equation equal to zero. Then,

$$\Phi(y) = \frac{\rho-c}{\rho+h} \Rightarrow \rho > c,\ 0 < \frac{\rho-c}{\rho+h} < 1,\ \frac{d^2}{dy^2}M(y) = (h+\rho)\Phi(y) > 0.$$

The optimum policy will be to place no order if $x > s$. If $x < s$, then place an order for $s-x$ items. Now, let's add a start-up cost to the example above. Call the start-up cost k. E(total cost) = T(y)=k + M(y) with an order, and M(x) without ordering. The policy is if the savings $M(x) - M(s) > k$, then place an order. Otherwise, do not place an order. The policy is if $x < s$ then order $S - x$; otherwise do not order. This is called the *(s,S) policy.*

Example: $c = 50$, $\rho = 110$, $h = -20$. D is normal with mean 100 and standard deviation of 15.

$$\Phi(s) = P(D \le S) = \frac{\rho-c}{\rho+h} = \frac{110-50}{110-20} = \frac{60}{90} = \frac{2}{3},\ P\left(\frac{D-100}{15} \le \frac{S-100}{15}\right) = \frac{2}{3}.$$

Using a table, $\frac{S-100}{15} = 0.43$. Therefore, $S = 106.45$.

Example: Use the same example above. This time D is uniform on [80,120].

$$\Phi(y) = \begin{cases} 0, & \text{for } y < 80. \\ \frac{1}{40}(y-80), & \text{for } 80 \le y \le 120 \\ 1, & \text{for } y > 120. \end{cases} \tag{5.8}$$

$$\frac{Y-80}{40} = \frac{2}{3} \Rightarrow y = 106.67.$$

Suppose there is a start-up cost of \$3,000. Use $x = 0$ to derive the total cost function.

$$M(y) = 50y - 20\int_{80}^{y} \frac{(y-z)}{40}\,dz + 110\int_{y}^{120} \frac{(z-y)}{40}\,dz = 50y - \frac{1}{2}\frac{(y-z)^2}{-2}\bigg|_{80}^{y} + \frac{11}{4}\frac{(z-y)^2}{2}\bigg|_{y}^{120} =$$

$$50y - \frac{1}{4}(y-80)^2 + \frac{11}{8}(120-y)^2 = M(107) + 3000 = 8400.13.$$

Therefore, $s = 55$.

5.5.3 A Stochastic Inventory

Suppose there is a stochastic pre-period and post-period. Use the previous example where $c = 50$, $\rho = 110$, $h = -20$, and Demand is uniform [80,120]. The optimum amount to order is $s = 107$. Let c and ρ be the same. Consider h above is a storage cost of 10 and a salvage value of 30. Let the holding cost for the first period be $h_1 = 10$, and for the second period be $h_2 = -20$. Demand D_1, D_2 are independent and uniform on [80,120]. Let $C_2^*(x_2)$ be the optimum choice from period two on-wards. It is the minimum cost for the second period if we have an inventory of x_2 at the start of the period. This is *optimized* for an order of $y_2^* - x_2$ where $y_2^* = 107$.

$$c_2(x_2, y_2) = 50(y_2 - x_2) + h_2\int_0^{\frac{1}{2}} (y_2 - z)\phi_2(z)\,dz + \rho\int_{\frac{1}{2}}^{\infty} (z - y_2)\phi_2(z)\,dz = 50(y_2 - x_2) + L_2(y_2).$$

$x_1 = 0$. Therefore,

$$c_1(0, y_1) = 50(y_1) + h\int_0^{y_1} (y_1 - z)\phi_1(z)\,dz + \rho\int_{y_1}^{\infty} (z - y)\phi_1(z)\,dz + c_2^*(x_2).$$

$y_1 \le 120$.

$$x_2 = y_1 - D_1 \le 120 - 80 = 40 =$$

$$50y_1 + \frac{10}{40}\int_0^{y_1} (y_1 - z)\,dz + \frac{110}{40}\int_{y_1}^{120} (z - y_1)\,dz + \frac{50}{40}\int_{80}^{120} (107 - [y_1 - z])\,dz + L_2(107).$$

The first integral is the holding cost, the second integral is the storage cost and the third integral is the cost per item. We want to make the best possible choice for the second period based on the first period which has already passed. This is called *dynamic programming*.

$$\frac{d}{dy}c_1(0, y_1) = 50 - \frac{1}{4}\int_{80}^{y_1} 1\,dz + \frac{11}{4}\int_{y_1}^{120} -1\,dz + \frac{5}{4}\int_{80}^{120} -1\,dz.$$

$$\frac{d}{dy_1}\left(\int_{80}^{y_1} (y_1 - z)\,dz\right) = (y_1 - y_1)\,\frac{dy_1}{dy_1} - (y_1 - 80)\,\frac{d80}{dy_1} + \int_{80}^{y_1} 1\,dz.$$

$$\frac{dc_1(0, y_1)}{dy} = 50 + \frac{y_1 - 80}{4} - \frac{11}{4}(120 - y_1) - \frac{5}{4}40 = 3y_1 - 350.$$

Set the derivative to zero to minimize $2y_1 - 350 = 0$. $Y_1 = 116\frac{2}{3} \approx 117$. Therefore, order 117 items in the first period and order 107 items in the second period. Suppose we have an infinite number of periods.

$$c^*(x) = \min_{y \geq x} \left[c(y-x) + h\int_0^y (y-z)\phi(z)\,dz + \rho\int_y^\infty (z-y)\phi(z)\,dz + \alpha\int_0^\infty c^*(y-z)\phi(z)\,dz \right].$$

α is a discounting factor between 0 and 1.

$$(1+i)S = k,\ S = \frac{k}{1+i} \Rightarrow \alpha = \frac{1}{1+i} < 1.$$

$$\frac{dc^*(x)}{dy} = c + h\int_0^y \phi(z)\,dz - \rho\int_y^\infty \phi(z)\,dz + \alpha\int_0^\infty \frac{\partial c^*(y-z)\phi(z)}{\partial y}\,dz =$$

$$c + h\Phi(y) - \rho(1-\Phi(y)) + \alpha\int_0^\infty -c\phi(z)\,dz = c + (\rho+h)\Phi(y) - \rho - \alpha c = (\rho+h)\Phi(y) - (\rho - c(1-\alpha)).$$

The optimum value of $\Phi(y)$ is

$$\Phi(y) = \frac{\rho - c(1-\alpha)}{\rho+h},\ y = \Phi^{-1}(\frac{\rho - c(1-\alpha)}{\rho+h}).$$

5.5.4 Inventory with Operating and Waiting Costs

The cost g(n) when there are n customers in the system. $E(C) = \sum_{n=0}^\infty g(n)P_n$, if the costs are linear(i.e. $g(n) = \beta$n), then $\sum_{n=0}^\infty \beta_n P_n = \beta\sum_{n=0}^\infty nP_n = \beta L$.

Example: Railroad cars are loaded by automatic equipment one at a time with unloading times exponential with mean $\frac{1}{\lambda}$. Arrivals are Poisson with mean rate λ. Cost of operating the machinery is $k\mu$. Demerge of a α per day must be paid on a car not unloaded by time C after arrival. What is the optimal choice of μ? There are three costs: Total cost(TC), Operating cost(OC),and Waiting cost(WC). TC = OC + WC. $E(TC) = E(OC) + E(WC) = k\mu + E(WC)$. E(WC)= E(number of arrivals)E(cost per arrival)= $\lambda E(h)W$ when

$$\begin{cases} 0, & \text{if } w \leq c. \\ \alpha(w-c), & \text{if } w > c \end{cases}$$

$M/M/1 \rightarrow P(W > t) = e^{-\mu(1-\rho)t} = e^{-(\mu-\lambda)t}$. $E(WC) = \lambda E(h(W)) = \lambda\int_0^\infty h(W)(\mu-\lambda)e^{-(\mu-\lambda)w}\,dw = \lambda\int_c^\infty \alpha(w-c)(\mu-\lambda)e^{-(\mu-\alpha)w}\,dw$. Let z=w-c. Then, $\lambda\alpha\int_0^\infty z(\mu-\alpha)e{-}(\mu-\alpha)(z+c)\,dz$. Integrate by parts. $\lambda\alpha e^{-c(\mu-\sigma)}E(W) = \lambda\alpha e^{-c(\mu-\lambda)}, \Rightarrow w = \frac{\lambda e^{-c(\mu-\lambda)}}{\mu-\lambda}$, $E(TC) = k\mu + \frac{\lambda\alpha e^{-c(\mu-\alpha)}}{\mu-\lambda}$. μ must be greater than λ. $\frac{dE(TC)}{du} = k - \lambda\alpha e^{-c(\mu-\lambda}[\frac{c}{\mu-\lambda} + \frac{1}{(\mu-\lambda)^2}] = k = v(u)$. v is decreasing. $\lim_{\mu\rightarrow\lambda+} v(\mu) = \infty$. $\lim_{\mu\rightarrow\infty} v(\mu) = 0$.

5.5.5 Inventory with Shortage Costs

The shortage cost per cycle is, $\rho\int_0^{\frac{v}{R-a}} I(t)\,dt + \int_{\frac{Q-v}{a}}^{\frac{Q}{a}} I(t)\,dt$. If m is the total cost per cycle, then $m = K + CQ + \frac{h}{2aR(R-a)}[(R-a)Q - vR]^2 + \frac{\rho Rv^2}{2a(R-a)}$. $T = \frac{m}{\frac{Q}{a}}$ which is the total cost per unit of time. $T = \frac{ka}{Q} + Ca + \frac{h}{Q2R(R-a)}[(R-a)Q - vR]^2 + \frac{\rho Rv^2}{2(R-a)Q}$. $\frac{\partial T}{\partial Q} = 0 = \frac{h(R-a)}{2R} - \frac{(h+\rho)R}{2(R-a)}\frac{v^2}{Q^2} - \frac{ka}{Q^2}$. $\frac{\partial T}{\partial v} = 0 = -h + \frac{(h+\rho)R}{(R-a)}\frac{V}{Q}$. Solve for $\frac{v}{Q}$: $\frac{v}{Q} = \frac{h(R-a)}{h+\rho}$, $Q^2 = \frac{2ka(h+\rho)R}{h\rho(R-a)}$. $Q = \sqrt{\frac{2ka(h+\rho)R}{h\rho(R-a)}}$. $v = \sqrt{\frac{2kah(R-a)}{\rho(h+\rho)R}}$. $g(x) = \int_{a(x)}^{b(x)} f(x,t)\,dt$. $\frac{dg(x)}{dx} = f(x,b(x))\frac{d(b(x))}{dx} - f(x,a(x))\frac{d(a(x))}{dx} + \int_{a(x)}^{b(x)} \frac{\partial f(x,t)}{\partial x}\,dt$. Consider a single cycle inventory with holding cost h per item at the end of the cycle. There is a shortage cost of ρ per item short at the end of the cycle. Each item costs an amount C. Demand D is random with density Φ. Demand is total demand for the cycle. Order an amount $y-x$ if x is the quantity on hand. Total costs are,

$$C(y-x)+h\left\{\begin{array}{ll}(y-D), & \text{for } D\leq y\\ 0, & \text{for } D>y\end{array}\right\}+\rho\left\{\begin{array}{ll}(D-y), & \text{for } D>y\\ 0, & \text{for } D\leq y\end{array}\right\}$$

The expected total cost is,

$$C(y-x)+h\int_0^y (y-z)\Phi(z)\,dz+\rho\int_y^\infty (z-y)\Phi(z)\,dz.$$

5.5.6 Summary

- Given a uniform demand for a product and shortages not permitted, the cost per cycle is

  $$\left\{\begin{array}{ll}0, & \text{for } Q=0\\ \text{k+CQ}, & \text{for } Q>0\end{array}\right.$$

  The total cost per unit of time is, $T=\frac{ak}{Q}+ac+\frac{hQ}{2}$. The optimal quantity is, $Q^*=\frac{dt}{dq}=\sqrt{\frac{2ak}{h}}$. The time taken to draw the optimal Q^* is, $t^*=\frac{Q^*}{a}=\sqrt{\frac{2k}{ah}}$. Given a uniform demand and shortages permitted, $T=\frac{ak}{Q}+ac+\frac{hs^2}{2Q}+\frac{(Q-s)^2}{2Q}$. $S^*=\sqrt{\frac{2ak}{h}}\sqrt{\frac{\rho}{\rho+r}}$, $Q^*=\sqrt{\frac{2ak}{h}}\sqrt{\frac{\rho+h}{\rho}}$, $t^*=\frac{Q^*}{a}=\sqrt{\frac{2k}{ah}}\sqrt{\frac{\rho+h}{\rho}}$. The maximum storage is Q^*-S^*. The fraction of time of no shortage is $\frac{\rho}{\rho+h}$.

- Given a uniform distribution, quantity discounts, and no shortages, compute $T_j=\frac{ak}{Q}+ac_j+\frac{hQ}{2}$, for $j=1,2,3,....$ Plot T_j vs Q. Use the curve closest to the x-axis to find the optimal policy.

- Stochastic models with a single period and no set-up costs. The optimal quantity to order is, $\Phi(y^0)=\frac{\rho-c}{\rho+h}$, where Φ is the cdf of demand. Solve for y^0.

- The stochastic model with an initial stock level of x is,

  $$y=\left\{\begin{array}{ll}y^0-x, & \text{if } x<y^0\\ 0, & \text{if } x\geq y^0\end{array}\right.$$

  $$\Phi(y^0)=\frac{\rho-c}{\rho+h}.$$

- Given a stochastic model with non-linear penalty costs,

  $L(y)=$ Expected shortage cost plus the holding cost.

  $$L(y)=\int_y^\infty \rho[\xi-y]f(\xi)d\xi+\int_0^y h[y-\xi]f(\xi)d\xi$$

  The total expected cost is $C(y-x)+L(y)$. The optimal policy is

  $$\left\{\begin{array}{ll}y^0, & \text{if } x<y^0\\ 0, & \text{if } x\geq y^0\end{array}\right.$$

  Note that y^0 satisfies $\frac{\partial(L(y))}{\partial y}+C=0$.

- Given a stochastic model with a single period and with setup costs,

$$T = \begin{cases} k + c(y - x) + L(y), & \text{if } y > x \\ L(x), & \text{if } y = x \end{cases}$$

$$L(y) = \rho \int_y^{\infty} (\xi - y)\Phi(\xi)\partial\xi + h \int_0^y (y - \xi)\Phi(\xi)\partial\xi$$

The optimal policy for ordering is

$$\begin{cases} S, & \text{if } x < s \\ 0, & \text{if } x \geq s \end{cases}$$

where $\Phi(S) = \frac{\rho - c}{\rho + h}$ and s satisfies $cs + L(s) = k + cS + L(S)$. This is called the (s, S) *policy.*

5.5.7 Homework and Answers

Do problems 1, 5, 7, 18, 20, 21((d) refers to (c)), 23, 24, 25, 26, 28, 29.

Problem 1: Suppose that the demand for a product is 30 units per month, and the items are withdrawn uniformly. The setup cost each time a production run is made is \$15. The production cost is \$1 per item, and the inventory holding cost is \$0.30 per item per month.

1. Assuming shortages are not allowed, determine how often to make a production run and what size it should be.

2. If shortages cost \$3 per item per month, determine how often to make a production run and what size it should be.

It is given that a=30, k=15, c=1, and h=0.3.

1. $Q = \sqrt{\frac{2(30)15)}{0.3}} = 54.77$. $t = \frac{Q}{a} = \frac{54.77}{30} = 1.83$.

2. p=3. $Q = \sqrt{\frac{2(30)(15)}{0.3}}\sqrt{\frac{3.3}{3}} = 57.45$. $t = \frac{Q}{a} = 1.91$.

Problem 5: A taxi company uses gasoline at the rate of 8,500 gallons/month. the gasoline costs \$1.05/gallon, with a setup cost of \$1,000. The inventory holding cost is 1 cent/gallon/month.

1. Assuming shortages are not allowed, determine how often and how much to order.

2. If shortages cost 50 cents/gallon/month, determine how often and how much to order.

It is given that a=8500, c=1.05, k=1000, h=0.01.

1. $Q = \sqrt{\frac{2(8500)(1000)}{0.01}} = 41231.06$. $t = \frac{Q}{a} = 4.85$.

2. p=0.5. $Q = \sqrt{\frac{2(8500)(1000)}{0.01}}\sqrt{\frac{0.51}{0.5}} = 41641.33$. $t = \frac{Q}{a} = 4.9$.

Problem 7: Solve problem 5(a) if the cost of gasoline is \$1.20/gallon for the first 20,000 gallons purchased, \$1.10 for the next 20,000 gallons, and \$1.00/gallon thereafter.

Let M be the cost per cycle and T the cost per unit of time. $T = \frac{Ma}{Q}, 0 \leq Q \leq 20,000$. $M = 1000 + 1.2Q + \frac{0.01}{2(8500)}Q^2$.

$$T = \frac{(1000)(8500)}{Q} + 1.2(8500) + \frac{(0.01)(8500)}{2(8500)}Q.$$

$$T' = -\frac{(1000)(8500)}{Q^2} + 0.005 < 0, Q \leq 20,000.$$

For $20,000 \leq Q \leq 40,000$, $M = 1000 + (1.2)(20,000) + (1.1)(Q - 20,000) + \frac{0.01Q}{2(8500)}$.

$$T = -\frac{(3000)(8500)}{Q^2} + 0.005 < 0, Q \leq 40,000.$$

For $40,000 < Q$, $M = 1000 + (1.2)(20,000) + (1.1)(20,000) + (1.0)(Q - 40,000) + \frac{0.01Q^2}{2(8500)}$.

$$T = \frac{(7000)(8500)}{Q} + (1.0)(8500) + 0.005Q.$$

$$T' = -\frac{(7000)(8500)}{Q^2} + 0.005 = 0, Q = \sqrt{\frac{(7000)(8500)}{0.005}} = 109,087.$$

$$t = \frac{Q}{a} = 12.834.$$

Problem 18: Consider a situation where a particular product is produced and placed in in-process inventory until it is needed in a subsequent production process. The number of units required in each of the next two months, as well as the setup cost, holding cost(charged as a function of excess of supply over requirement and charged at the end of the period), and regular-time unit production cost, are as follows:

Month	Requirement	Setup Cost(\$)	Holding Cost(\$)	Unit Cost(\$)
1	3	5	0.30	9
2	4	5	0.30	9

Determine the optimal production schedule that satisfies the monthly requirements. Use the algorithm presented in Section 18.3 of the text book.

x_3/z_3	0	1	2	3	4	C_3^*	z_3^*
0					47	47	4
1				36		36	3
2			27			27	2
3		18				18	1
4	4					4	0

x_2/z_2	0	1	2	3	4	C_2^*	z_2^*
0				87	90	87	3
1			77	78	83	77	2
2		67	68	71	76	67	1
3	47	58	61	64	64	47	0
4	38	51	54	52		38	0

x_1/z_1	0	1	2	3	4	C_1^*	z_1^*
1	87	92	92	82	85	82	3

Produce 3 at the start of the first period, none in the second period, and 4 at the start of the third period.

Problem 20: A newspaper stand purchases newspapers for 18 cents and sells them for 25 cents. The shortage cost is 25 cents per newspaper(because the dealer buys papers at retail price to satisfy shortages). The holding cost is 0.1 cent. The demand distribution is a uniform distribution between 200 and 300. Find the optimal number of papers to buy.

$$\Phi(y) = \frac{y-200}{100} = \frac{p-c}{p+h} = \frac{25-18}{25+0.01} = \frac{7}{25.01},\ y = 200 + \frac{700}{25.01} \approx 228 = S.$$

Problem 21: Suppose the demand D for a spare airplane part has an exponential distribution with parameter $\frac{1}{50}$. That is,

$$\varphi_D(\xi) = \begin{cases} \frac{1}{50}e^{-\frac{\xi}{50}}, & \xi \geq 0. \\ 0, & \text{otherwise.} \end{cases}$$

This plane will be obsolete in 1 year, hence all production is to take place at the present time. The production costs now are \$1,000 per item — that is, c = 1,000 — but they become \$10,000 per item if they must be supplied at later dates — that is, p = 10,000. The holding costs, charged on the excess after the end of the period, are \$300 per item.

1. Determine the required number of spare parts.
2. Suppose that the manufacturer has 23 parts already in inventory(from a similar, but now obsolete airplane). Determine the optimal inventory policy.
3. Suppose that p cannot be determined now, but the manufacturer wishes to order a quantity so that the probability of a shortage equals 0.05. How many units should be ordered?
4. If the manufacturer were following an optimal policy, but ordered the quantity in part (b), what is the implied value of p?

$$\Phi_D(z) = 1 - e^{-\frac{3}{50}}, z \geq 0.$$

1. $\Phi_D(s) = \frac{p-c}{p+h} = \frac{10{,}000-1{,}000}{10{,}000+300} = \frac{9{,}000}{10{,}300} = 1 - e^{-\frac{s}{50}}$, $s = -50\ln(\frac{13}{103}) = 103.49 \approx 103.$
2. Since $23 < S$, order up to s, that is order 80.
3. $0.05 = P(D > S) = e^{-\frac{s}{50}}$, $s = -50\ln(0.05) = 149.79 \approx 150.$
4. $\frac{p-1000}{p+300} = \Phi_D(150) = 1 - e^{-\frac{150}{50}} = 1 - e^{-3} = 0.95; p = 25,700.$

Problem 23: A student majoring in operations research enjoys optimizing his personal decisions. He is analyzing on such decision currently, namely how much money to take out of his savings account(if any) to buy traveler's checks before leaving on a summer vacation trip to Europe.

He already has used the money he had in his checking account to buy traveler's checks worth \$1,200, buy this may not be enough. In fact, he has estimated the probability distribution of what he will need as shown in the following table:

Amount($)	1000	1100	1200	1300	1400	1500	1600	1700
Probability	0.05	0.10	0.15	0.25	0.20	0.10	0.10	0.05

If he turns out to have less than he needs, then he will have to leave Europe 1 week early for every $100 short. Because he places a value of $150 on each week in Europe, each week lost would thereby represent a net imputed loss of $50 on him. However, every $100 traveler's check costs an extra $1. Furthermore, each such check left over at the end of the trip(which would be redeposited in the saving account) represents a loss of $2 in interest that could have been earned in the savings account during the trip, so he does not want to purchase too many.

Using these data, determine the optimal decision on how may additional $100 traveler's checks(if any) the student should purchase from his savings account money. The amount needed is D.

D	1000	1100	1200	1300	1400	1500	1600	1700
Φ_D	0.05	0.10	0.15	0.25	0.20	0.10	0.10	0.05
Φ_D	0.05	0.15	0.30	0.55	0.75	0.85	9.95	1.00

$$p = 50,\ c = 1,\ h = 2,\ \Phi(s) = \frac{50-1}{50+2} = \frac{49}{52} = 0.94.$$

Choose s=1600 so buy 4 additional $100 checks.

Problem 24: Find the optimal ordering policy for a one-period model, where the demand has a probability density,

$$\varphi_D(\xi) = \begin{cases} \frac{1}{20}, & 0 \leq \xi \leq 20 \\ 0, & \text{otherwise} \end{cases}$$

and the costs are holding cost = $1 per item, shortage cost = $3 per item, setup cost = $1.50 per item, and Production cost = $2 per item.

$$\frac{s}{20} = \Phi(S) = \frac{3-2}{3+1} = \frac{1}{4},\ s = 5.$$

$$M(y) = 2y + 1\int_0^y (y-z)\frac{1}{20}\,dz + 3\int_y^{20}(z-y)\frac{1}{20}\,dz = 2y - \left.\frac{y-z}{40}\right|_0^y + \left.\frac{3}{40}(z-y)^2\right|_y^{20} =$$

$$2y + \frac{y^2}{40} + \frac{3}{40}(20-y)^2 = \frac{1}{10}[y^2 - 10y + 300].$$

$$M(5) = \frac{1}{10}[25 - 50 + 300] = 27.5, k = 1.50,\ 29 = M(s) = \frac{1}{10}[s^2 + 10s + 300],\ s^2 - 10s + 10 = 0,$$

$$s = \frac{10 + -\sqrt{100-40}}{2} = 5 + -\sqrt{15}.$$

So $s = 5 - \sqrt{15} = 1.13$. Use (s,S) system with s=1.13, and S=5.

Problem 25: The campus bookstore must decide how many textbooks to order for a course that will be offered only once. The number of students who will take the course is a random variable D, whose distribution can be approximated by a (continuous) uniform distribution on the interval [40,60]. After the quarter starts, the value of D becomes known. If D exceeds the number of books available, the known shortfall is made up by placing a rush order at a cost of \$14 plus \$2 per book over the normal ordering cost. If D is less than the stock on hand, the extra books are returned for their original ordering cost less \$1 each. What is the order quantity that minimizes the expected cost?

Let c be the normal cost per book and $M(y)$ the total expected cost if y are ordered. Let D have density Φ.

$$M(y) = cy + (1-c)\int_0^y (y-z)\Phi(z)\,dz + 14\int_y^\infty \Phi(z)\,dz + (2+c)\int_y^\infty (z-y)\Phi(z)\,dz =$$

$$cy + \frac{(1-c)}{20}\int_{40}^y (y-z)\,dz + \frac{14}{20} + \frac{(2+c)}{20}\int_y^{60}(z-y)\,dz,\ M'(y) = c + \frac{(1-c)}{20}\int_{40}^y 1\,dz =$$

$$\frac{14}{20} = \frac{(2+c)}{20}\int_y^{60} 1\,dz = c + \frac{(1-c)}{20}(y-40) - 0.7 - \frac{(2+c)}{20}(60-y) = 0.15y - 8.7 = 0,$$

$$y = \frac{8.7}{0.15} = 58 \text{ min.}$$

Since $M''(y) > 0$.

Problem 26: Consider the following inventory model, which is a single- period model with known density of demand $\varphi_D(\xi) = e^{-\xi}, \xi > 0$, and zero elsewhere. There are two costs connected with the model: The first is the purchase cost, given by $c(y-x)$ and the second is the unsatisfied demand cost, which is just a constant, p(independent of the amount of unsatisfied demand).

1. If x units are available and goods are ordered up to y, write the expression for the expected loss, and describe completely the optimal policy.
2. If a fixed cost K is also incurred whenever an order is placed, describe the optimal policy.

$$T = C(y-x) = pP(D > y) = C(y-x) + pe^{-y}, y > x.$$

1. $\frac{dt}{dy} = c - pe^{-y} = 0, y = \ln\left[\frac{p}{c}\right].$

   $$\frac{d^2T}{dy^2} = pe^{-y} > 0.$$

   If $x < \ln\left[\frac{p}{c}\right]$, order up to $\ln\left[\frac{p}{c}\right]$.
2. Let $S = \ln(\frac{p}{c})$ and $s < S$ be such that T(s)=T(S)+k.

   $$C(s-x) + pe^{-s} = C(S-x) + pe^{-S} + k = c\left(\ln\left[\frac{p}{c}\right] - x\right) + p\frac{c}{p} + k = c\left(\ln\left[\frac{p}{c}\right] - x + 1\right) + k.$$

   $$s + \frac{p}{c}e^{-s} = \ln\left[\frac{p}{c}\right] + 1 + \frac{k}{c}.$$

   s is the smallest root of this equation. Use (s,S) policy.

Problem 28: There are production processes for which the difference between the cost of producing the maximum number of units allowed by some capacity restriction and the cost of producing any number of units less than this maximum is negligible; i.e. ordering is by batches. Consider a one-stage model, where the only two costs are holding costs given by

$$h(y-D) = \frac{3}{10}(y-D),$$

and the penalty cost of unsatisfied demand is given by,

$$\varphi_D(\xi) = \begin{cases} \frac{e^{-\frac{\xi}{25}}}{25}, & \xi \geq 0 \\ 0, & \text{otherwise} \end{cases}$$

If you order, you must order in batches of 100 units, and this quantity is delivered instantaneously. Thus, if x denotes the quantity on hand, and if you do not order, then $y = x$. If you order one batch, then $y = x + 100$. Let $G(y)$ denote the total expected cost of this inventory problem when there are y units available for the period(after you have ordered).

1. Write the expression for G(y).
2. What is the optimal ordering policy?

1.

$$G(y) = \frac{3}{10} \int_0^y (y-z) \frac{e^{-\frac{z}{25}}}{25}\, dz + 2.5 \int_y^{\infty} (z-y) \frac{e^{-\frac{z}{25}}}{25}\, dz =$$

$$\frac{3}{10}\left[-(y-z)e^{-\frac{z}{25}} \Big|_0^y - \int_0^y e^{-\frac{z}{25}}\, dz \right] + 2.5 \left[(z-y)e^{-\frac{z}{25}} \Big|_y^{\infty} + \int_y^{\infty} e^{-\frac{z}{25}}\, dz \right] =$$

$$0.3[y + 25e^{-\frac{z}{25}}|_0^y] + 2.5[-25e^{-\frac{z}{25}}|_y^{\infty}] = 0.3[y + 25e^{-\frac{y}{25}} - 25] + 2.5[25e^{-\frac{y}{25}}] = 0.3y + 70e^{-\frac{y}{25}} - 7.5.$$

2.

$$G'(y) = 0.3 - \frac{70}{25}e^{-\frac{y}{25}} = 0,\ e^{-\frac{y}{25}} = 0.1071,\ y = 55.8398.$$

We seek a value of $y < 55.8398$ where the cost with ordering equals the cost without ordering.

$$G(y) = G(y + 100).$$

$$0.3y + 70e^{-\frac{Y}{25}} - 7.5 = 0.3(y + 100) + 70e^{-\frac{y+100}{25}} - 7.5 = 70e^{-\frac{y}{25}}(1 - e^{-4}) = 30.$$

$$e^{-\frac{y}{25}} = \left(\frac{3}{7}\right) \frac{1}{1 - e^{-4}} = 0.4366, y = 20.7203.$$

Use a (k, Q) policy with $k = 21$ and $q = 100$. That is, order if the inventory is less than 21. Order one lot of 100.

Problem 29: Consider the following inventory situation. Demands are independent with common density given by the following:

$$\varphi_D(\xi) = \begin{cases} \frac{e^{-\frac{\xi}{25}}}{25}, & \xi \geq 0 \\ 0, & \text{otherwise} \end{cases}$$

Orders may be placed at the start of each period without setup cost at a price of $c = 10$. There are a holding cost of 6 per unit remaining in stock at the end of each period and a penalty cost of 15 unit quantity bocklogged.

1. Find the optimal one-period policy.
2. Find the optimal two-period policy.

$c = 10$, $h = 6$, $p = 15$.

1.

$$1 - e^{-\frac{y}{25}} = \Phi(y) = \frac{p-c}{p+h} = \frac{15-10}{15+6} = \frac{5}{21}.$$

$$y = -25\ln(\frac{16}{21}) = 6.7983.$$

2. Use equation on page 719 of the text book.

$$-15 + 21(1 - e^{-\frac{y}{25}}) - 5(1 - e^{-\frac{y-6.7983}{25}}) + 21\int_0^{y-6.7983} (1 - e^{-\frac{y-z}{25}})\frac{e^{-\frac{z}{25}}}{25}\, dz = 0$$

$$0 = 1 - e^{-\frac{y}{25}}(21 - 5e^{-\frac{6.7983}{25}}) + \frac{21}{25}\int_0^{y-6.7983} e^{-\frac{z}{25}}\, dz - \frac{21}{25}e^{-\frac{y}{25}}(y - 6.7983) =$$

$$22 - (36.2894 + 0.84y)e^{-\frac{y}{25}} = y = 23.2932.$$

Order up to 23.2932 in period 1 and up to 6.7983 at the start of period 2.

Problem 33: Solve problem 31 for an infinite-period model by using a discount factor of $\alpha = 0.90$.

$$1 - e^{-\frac{y}{25}} = \Phi(y) = \frac{p - c(1-\alpha)}{p+h} = \frac{2 - 1(1-0.9)}{2+0.25} = \frac{1.9}{2.25} = 0.84.$$

$$y = -25\ln(0.1556) = 46.5188.$$

Problem 36: A supplier of high fidelity receiver kits is interested in using an optimal inventory policy. The distribution of demand per month is uniform between 2,000 and 3,000 kits. The cost of each kit is \$150. The holding cost is estimated to be \$2 per kit per month, and the unsatisfied demand cost is \$30 per kit per month. Using a discount factor of $\alpha = 0.90$, find the optimal inventory policy for this "infinite" horizon problem.

$$\frac{y-2000}{1000} = \Phi(y) = \frac{p - c(1-\alpha)}{p+h} = \frac{30 - 150(1-0.90)}{30+2} = \frac{15}{32}.$$

$$y = \left(\frac{15}{32}\right)1000 + 2000 = 2468.75.$$

5.6 Forecasting

5.6.1 Moving Average and Exponential Smoothing

Let x_t be the observed value of some changing quantity at time t. Suppose $x_t = A + \epsilon_t$, where $\epsilon_1, \epsilon_2, ...$ are iid and have a mean of 0. A is a constant, and t is discrete values of time. We are given $x_1, x_2, ..., x_{10}$ and asked to predict $\hat{x}_{11}$. Then,

$$\hat{x}_{11} = E(x_1|x_1, ..., x_{10}) = E(A + \epsilon_{11}|x_1, ..., x_{10}) = A + E(\epsilon_{11}) = A + 0 = A \approx \hat{\mu}_{10}.$$

Estimate A and predict the value of ϵ_{11}. $A \approx \frac{1}{10}\sum_{i=1}^{10} x_i$ will be the estimate.

$$\frac{1}{10}\sum_{i=1}^{10} x_i = \hat{\mu}_{10} = \hat{x}_{11}.$$

If we think that A may be slowly changing with no information on how, then the above can be replaced by a *moving average.* $\hat{\mu}_t = \frac{1}{n}\sum_{i=0}^{n-1} x_{t-i}$, which takes the most recent values of x. $\hat{\mu}_{t+1} = \hat{\mu}_t$. Alternatively, use small weights on the old data and heavier weights on the more recent data. The equation follows.

$$\hat{\mu}_n = \frac{\sum_{j=0}^{n-1}\alpha^j x_{n-j}}{\sum_{j=0}^{n-1}\alpha^j}, 0 < \alpha < 1.$$

$$\frac{\sum_{j=0}^{n-1}\alpha^j x_{n-j}}{\sum_{j=0}^{n-1}\alpha^j} = \frac{\sum_{j=0}^{n-1}\alpha^j x_{n-j}}{\frac{1-\alpha^n}{1-\alpha}} = \left(\frac{1-\alpha}{1-\alpha^n}\right)\sum_{j=0}^{n-1}\alpha^j x_{n-j} \approx (1-\alpha)\sum_{j=0}^{n-1}\alpha^j x_{n-j},$$

because $\alpha^n \approx 0$. So,

$$(1-\alpha)x_n + (1-\alpha)\sum_{j=1}^{n-1}\alpha^j x_{n-j}.$$

Let,

$$\hat{\mu}_n = (1-\alpha)\sum_{j=0}^{n-1}\alpha^j x_{n-j} = (1-\alpha_n)x_n + \alpha(1-\alpha)\sum_{j=1}^{n-1}\alpha^{j-1}x_{n-j}.$$

Let $i = j-1$. So that,

$$(1-\alpha)x_n + \alpha(1-\alpha)\sum_{j=0}^{n-2}\alpha^j x_{n-(j+1)} = (1-\alpha)x_n + \alpha(1-\alpha)\sum_{j=0}^{n-2}\alpha^j x_{(n-1)-i} = \hat{\mu}_n = (1-\tilde{\alpha})x_n + \tilde{\alpha}\hat{\mu}_{n-1}.$$

In the text book, the equation is $\tilde{\alpha}x_n + (1-\tilde{\alpha})\hat{\mu}_{n-1}$. This is called *exponential smoothing.* $\tilde{\alpha} = 1-\alpha$. So, $\hat{\mu}_n = \hat{x}_{n+1}$ which is the prediction. Suppose that x_t is such $x_t = A_t + \epsilon_t, A_t = A_{t-1} + B$ which is linear with slope B. Then, the estimator and predictor are not the same.

$$\hat{\mu}_t \approx A_t,\ x_{t+1} = A_{t+1} + \epsilon_{t+1} = A_t + B + \epsilon_{t+1},\ E(x_{t+1}) = E(A_t) + E(B) + E(\epsilon_{t+1}).$$

Let $\hat{B}_t$ be the estimate of the trend. $\hat{B}_t \approx B$. Then,

$$\hat{x}_{t+1} = E(A_{t+1} + \epsilon_{t+1}) = E(A_t) + E(B) + E(\epsilon_{t+1}) = \hat{\mu}_t + \hat{B}_t.$$

So,

$$x_{t+4} = A_{t+4} + \epsilon_{t+4} = A_{t+3} + B + \alpha_{t+4} = ... = A_t + 4B + \epsilon_{t+1}.$$

$$\hat{x}_{t+4} = E(x_{t+4}) = E(A_t) + 4E(B) + E(\epsilon_{t+4}) = \hat{\mu}_t + 4\hat{B}_t.$$

5.6.2 Cyclical Trend Analysis

Let $x_n = A + \epsilon_n$, where ϵ_n's are independent with mean 0. $\frac{1}{n}\sum_{i=0}^{n-1} x_{n-i}$ is one scheme to find A. $\alpha(x_n) + (1-\alpha)\hat{\mu}_{n-1}$ is another scheme to find A. $\hat{\mu}_n$ is an estimator of the mean of A. $\hat{x}_{n+1}$ is a predictor of x_{n-1}.

$$E(x_n) - E(x_{n-1}) = B,\ x_n = A + (n-1)B + \epsilon_n,\ \hat{\mu}_n = \alpha x_n + (1-\alpha)(\hat{\mu}_{n-1} + \hat{B}_{n-1}).$$

$$\hat{B}_n = \beta(\hat{\mu}_n - \hat{\mu}_{n-1}) + (1-\beta)\hat{B}_{n-1},\ \hat{x}_{n+1} = \hat{\mu}_n + \hat{B}_n,\ \hat{x}_{n+m} = \hat{\mu}_n + m\hat{B}_n.$$

Look at $\frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{x}_i)^2$ to guide the predictor process.

Example:

year	miles flown(1000's)	$\frac{1}{2}\sum_{i=0}^{2} x_{n-i} = \hat{\mu}_n$
1963	99603	—
1964	106192	—
1965	115431	107075.33
1966	119154	113592.33
1967	126515	120366.67
1968	128975	124881.33
1969	143664	133051.33
1970	157497	143378.67

$x_n - \hat{x}_n$ are called *residual values.*

$$\frac{1}{5}\sum_{i=1966}^{1970}(x_i - \hat{x}_i)^2 = 26747497.67.$$

Look at the example with a trend. Let $E(x_n) - E(x_{n-1}) = \beta$. Then,

$$\hat{\mu}_n = 0.2x_n + 0.8(\hat{\mu}_{n-1} + \hat{B}_{n-1}),\ \hat{B}_n = 0.1(\hat{\mu}_n - \hat{\mu}_{n-1}) + 0.9\hat{B}_{n-1},\ \hat{x}_{n+1} = \hat{\mu}_n + \hat{B}_n.$$

So,

year	$\hat{\mu}_n$	$\hat{B}_n$	$\hat{x}_{n+1}$	$x_n - \hat{x}_n$
1963	99603	7000(guess)	106603	—
1964	106520.8	6991.78	113512.58	—
1965	113896.26	7030.15	120926.41	—
1966	120571.93	6994.70	127566.63	-1772.41
1967	—	—	—	-1051.63
1968	—	—	—	-5354.97
1969	—	—	—	3538.45
1970	—	—	—	9726.43

$$\frac{1}{5}\sum_{i=1966}^{1970}(x_i - \hat{x}_i)^2 = 28009427.10.$$

The trend analysis seems to have been the better method since 28009427.10 > 26747497.67. Suppose we have $x_1, x_2, x_3, x_4, x_5, x_6, x_7$. $x_n = AI_n + \epsilon_n$ where ϵ_n's are independent with a mean of 0. The cyclical approach to Forecasting follows:

$$\hat{\mu}_n = \alpha\left(\frac{x_n}{\hat{I}_{n-p}}\right) + (1-\alpha)\hat{\mu}_{n-1}.$$

p is the period.

$$\hat{I}_n = \beta\left(\frac{x_n}{\hat{\mu}_n}\right) + (1-\beta)\hat{I}_{n-p}.$$

Again, we can use residual to get an idea of how good we are predicting. Beware of plugging in numbers. You must interpret notation according to seasons.

$$\hat{x}_{n+1} = \hat{\mu}_n \hat{I}_{(n+1)-p},\ \hat{x}_{n+m} = \hat{\mu}_n \hat{I}_{(n+m)-p}.$$

Let's say we have a run under cyclical conditions. Let I be the seasonal factor.

$$x_n = AI_{n-p} + \epsilon_n.$$

We must find A and the subscript $n-p$.

$$\hat{\mu}_n = \alpha\left(\frac{x_n}{\hat{I}_{n-p}}\right) + (1-\alpha)(\hat{\mu}_{n-1}\hat{I}_{n-p}),\ \hat{I}_n = \beta\left(\frac{x_n}{\hat{\mu}_n}\right) + (1-\beta)\hat{I}_{n-p},\ \hat{x}_{n+1} = \hat{\mu}_n \hat{I}_{n-p+1}.$$

Example:

year	1	2
winter	28.461	26.718
spring	30.369	29.869
summer	32.750	32.953
fall	30.382	29.974

$$28.461 + 30.369 + 32.750 + 30.382 = 121.962.$$

$$\hat{\mu}_1 = \frac{121.962}{4} = 30.491,\ \hat{I}_1 = \frac{28.461}{30.369} = 0.933,\ \hat{I}_2 = \frac{30.369}{30.491} = 0.996,\ \hat{I}_3 = 1.074,\ \hat{I}_4 = 0.996.$$

Replace the previous set of $\hat{I}_n$ terms in the third column.

year 2	$\hat{\mu}_n$	$\hat{I}_n$
winter	30.117	0.924
spring	30.092	0.995
summer	30.209	1.077
fall	30.184	0.996

year 5	μ_n	I_n
winter	28.394	0.854
spring	28.708	1.021
summer	28.739	1.130
fall	29.033	0.966

$A = 30; \alpha = \beta = 0.2.$. The true seasonal factors are $I_1 = 0.7; I_2 = 1.1; I_3 = 1.2; I_4 = 0.9$. $\epsilon \sim uniform(-5, 5)$.

5.6.3 Summary

- *Last value,*

$$F_{t+1} = x_t,\, x_t = A + e_t.$$

- *Average Forecasting,*

$$F_{t+1} = \frac{1}{t}\sum_{i=1}^{t} x_i.$$

- *Moving average,*

$$F_{t+1} = \frac{1}{n}\sum_{i=t-n+1}^{t} x_i.$$

- *Exponential smoothing,*

$$F_{t+1} = \alpha x_t + (1-\alpha)F_t,$$

or

$$F_{t+1} = F_t + \alpha(x_t - F_t).$$

The drawback is that it lags behind in predicting trends of some periods.

- *Linear trend,*

$$S_t = \alpha x_t + (1-\alpha)(S_{t-1} + B_{t-1}),\, B_1 = \beta(S_t - S_{t-1}) + (1-\beta)B_{t-1},\, F_{t+m} = S_T + mB_t,$$

where m is the number of periods to forecast ahead.

- *Seasonal effects(reference p. 752 of textbook),*

$$S_t = \alpha\frac{x_t}{I_{t-\rho}} + (1-\alpha)S_{t-1},$$

ρ periods ahead.

$$I_t = \gamma\frac{x_t}{S_t} + (1-\gamma)I_t + -\rho,\, F_{t+m} = S_t I_{t-\rho+m}.$$

- *Forecasting errors,*

$$E_t = x_t - F_t.$$

The *mean square error(mse)* is

$$MSE = \frac{E_1^2 + E_2^2 + E_3^2 + ... + E_n^2}{n}.$$

5.7 Markov Decision Making

5.7.1 Policy Making

Start with decisions as opposed to states. The decisions are 1,...,m. A *policy* R is a function with domain 1,...,n and range in 1,...,m. $P_{ij}^{(R(i))} = p_{ij}^{(R)}$. IP$(R) = [p_{ij}(R(i))]$ is the transition matrix for the chain given by policy R.

Example: Demand for power has states 1,2 and the following transition matrix:

$$\mathrm{IP} = \begin{array}{c|cc|} & 1 & 2 \\ \hline 1 & \frac{3}{4} & \frac{1}{4} \\ 2 & \frac{3}{4} & \frac{1}{4} \end{array}$$

The states are as follows:

1= demand of 1 and generator running;
2 = demand of 2 and generator running;
3 = demand of 1 and buying power;
4 = demand of 2 and buying power;

The decisions are as follow:

1 = run the generator;
2 = buy power;

R(1)= 1, R(2)= 2, R(3)= 2, R(4)= 1.

What would be a good policy? Let $q_{ij}(k)$ be the expected cost of going from state i to state j in 1 step under decision k. C_{ik} is the expected cost of being in state i and making decision k.

$$c_{ik} = \sum_{i=1}^{n} p_{ij}(k) q_{ij}(k).$$

Consider the generator problem with $R_1(1) = 1, R_1(2) = 1, R_1(3) = 2, R_1(4) = 1.$

$$\mathrm{IP}(R) = \begin{array}{c|cccc|} & 1 & 2 & 3 & 4 \\ \hline 1 & \frac{3}{4} & \frac{1}{4} & 0 & 0 \\ 2 & \frac{1}{4} & \frac{3}{4} & 0 & 0 \\ 3 & 0 & 0 & \frac{3}{4} & \frac{1}{4} \\ 4 & 0 & 0 & \frac{1}{4} & \frac{3}{4} \end{array}$$

We are given that P(demand stays the same)=$\frac{3}{4}$ and P(demand changes)=$\frac{1}{4}$.

$$C(R_1) = \begin{vmatrix} 6 \\ 6 \\ 5 \\ 7 \end{vmatrix}$$

$$G(R)\tilde{I} = C(R) + (\mathrm{IP}(R) - I)V(R).$$

The equations are:

$$g(R_1) = C_1(R) + (\mathrm{IP}_{11}(R_1) - 1)V_1(R_1) + \mathrm{IP}_{13}(R_1)V_3(R_1) + \mathrm{IP}_{14}(R_1)0.$$

$$g(R_1) = 6 - \frac{1}{4}V_1(R) + \frac{1}{4}V_2(R).$$

Note that

$$I = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{vmatrix}$$

$$g(R_1) = 6 + \frac{1}{4}V_1(R_1) - \frac{1}{4}V_2(R_1) + 0,\ g(R_1) = 5 - \frac{1}{4}V_1(R_1),\ g(R_1) = 7 + \frac{1}{4}V_1(R_1) + \frac{3}{4}V_2(R_1).$$

Solve the above 4 equations and get:

$$g = 6,\ V_1 = -1,\ V_2 = -1,\ V_3 = -4,\ V_4 = 0.$$

The next step is to try to improve each state.

$$\tilde{I}g(R) = C(R) + [\mathrm{IP}(R) - I]V(R).$$

The V_i's are costs. So large negative numbers are desirable. Optimize the following:

State 1:

$$g = 6 - \frac{1}{4}V_1 + \frac{1}{4}V_2.$$

$$k = 1 : 6 - \frac{1}{4}(-1) + \frac{1}{4}(-1) = 6.$$

$$k = 2 : C_{12}(0-1)V_1 + \frac{3}{4}V_3 + \frac{1}{4}V_4 = 5 - 1(-1) + \frac{3}{4}(-4) = 3.$$

$R_2(1) = 2$ based on the above values. This is called the *policy improvement step.*

State 2:

$$g = C_{21} + \frac{1}{4}V_1 + \left(\frac{3}{4} - 1\right)V_2 =$$

$$k = 1 : 6 + \frac{1}{4}(-1) - \frac{1}{4}(-1) = 6.$$

$$k = 2 : C_{22} - 1V_2 + \frac{1}{4}V_3 = 7 - 1(-1) + \frac{1}{4}(-4) = 7.$$

$$p_{2j}(2) = \left[0, 0, \frac{1}{4}, \frac{3}{4}\right].$$

Therefore, $R_2(2) = 1$.

State 3:

$$k = 2 : g = 6.$$

$$k = 1 : C_{31} + \frac{3}{4}V_1 + \frac{1}{4}V_2 - V_3 = 7 + \frac{3}{4}(-1) + \frac{1}{4}(-1) - (-4) = 7.$$

$$P_{3j}^{(1)} = \left[\frac{3}{4}, \frac{1}{4}, 0, 0\right].$$

Therefore, $R_2(3) = 2$.

State 4:

$$k = 1 : g = 6.$$

$$k = 2 : C_{42} + \frac{1}{4}V_3 - \frac{1}{4}V_4 = 7 + \frac{1}{4}(-4) - 0 = 6.$$

$$P_{4j}^{(2)} = \left[0, 0, \frac{1}{4}, \frac{3}{4}\right].$$

Therefore, $R_2(4) = 1$.

Now, let's start over with policy R_2. $R_2(1) = 2, R_2(2) = 1, R_2(3) = 2, R_2(4) = 1$. $g = 5 - V_1 + 0V_2 + \frac{3}{4}V_3 + \frac{1}{4}V_4$, $g = 6 - \frac{1}{4}V_1 - \frac{1}{4}V_2$, $g = 5 - \frac{1}{4}V_3 + \frac{1}{4}V_4$, $g = 7 + \frac{1}{4}V_1 + \frac{3}{4}V_2 - V_4$.

Solve the above system for: $V_1 = -\frac{5}{2}, V_2 = -1, V_3 = -\frac{5}{2}, V_4 = 0$. $g = 5\frac{5}{8}$. $R_3(1) = 2, R_3(2) = 1, R_3(3) = 2, R_3(4) = 1$. When the policies remain the same, the optimal policy is established. An alternate way of finding the optimal policy is as follow: $V^n(R) = \sum_{n=0}^{N-1} \mathrm{IP}(R)C(R)$.

$$V^N(R) = \sum_{n=0}^{N-1} \alpha^n \mathrm{IP}^N(R)C(R) = C(R) + \sum_{n=1}^{N-1} \alpha^n \mathrm{IP}^N(R)C(R) = C(R) + \alpha\mathrm{IP}(R)\sum_{n=0}^{N-1} \alpha^{n-1}\mathrm{IP}^{n-1}C(R) =$$

Let $s = n - 1$. $V^N(R) = C(R) + \alpha\mathrm{IP}(R)\sum_{s=0}^{N-2} \alpha^s \mathrm{IP}^s(R)C(R) = C(R) + \alpha\mathrm{IP}(R)V^{N-1}(R)$, and it will converge when we take the limits. $V(R) = \lim_{N\to\infty} V^N(R) = C(R) + \alpha\mathrm{IP}(R)V(R)$. $0 = C(R) + [\alpha\mathrm{IP}(R) - I]V(R)$. Then, use the policy improvement scheme. Solve the system. $V_1(R_1) = 30, V_2(R_1) = 30, V_3(R_1) = 28, V_4(R_1) = 31$.
State 1:

$$dec1 : V_1 = 30,$$

$$dec2 : V_1 = 5 + \frac{4}{5}\left[\frac{3}{4}(28) + \frac{1}{4}(31)\right] = 28.$$

Therefore, let $R_2(1) = 2$.

State 2:

$$dec1 : V_2 = 30,$$

$$dec2 : V_2 = 7 + \frac{4}{5}\left[\frac{1}{4}(28) + \frac{3}{4}(31)\right] = 31.2.$$

Therefore, let $R_2(2) = 1$. $R_2(1) = 2, R_2(2) = 1, R_2(3) = 2, R_2(4) = 1$, which is optimal. $q_{ij}(k)$ is the expected one step cost of going from i to j if we make decision k. $C_{ik} = \sum_{j=1}^m P_{ij}(k)q_{ij}(k)$. That is the one step cost of being in state i and making decision k. The cost of the n-th step is $P^{(n)}(R)C(R)$. The cost of the initial state and the first n-1 steps is $V^N(R) = \sum_{n=0}^{N-1} \mathrm{IP}^{(N)}C(R)$. $\Pi(R) = [\Pi_1(R), \Pi_2(R), ..., \Phi_m(R)]$. $\sum_{j=1}^m \Pi(j)C_jR(j)$ is the expected long run one step cost. It is also equal to $\Pi(R)C(R) = g(R)$. Let C_{ik} be the expected cost of being in state i and making decision k.

$$C(R) = \begin{vmatrix} C_1R(1) \\ . \\ . \\ . \\ C_MR(m) \end{vmatrix}$$

$$V^N(R) = \sum_{n=0}^{N-1} \mathrm{IP}^n(R)C(R),\ g(R) = \Pi(R)C(R).$$

Let,

$$\tilde{I} = \begin{vmatrix} 1 \\ 1 \\ 1 \\ . \\ . \\ . \\ 1 \end{vmatrix}$$

$\in m$ is 1's, and $V(R) = \sum_{n=0}^{\infty}[\mathrm{IP}^n(R) - \tilde{I}\Pi(R)]C(R)$. The difference of the two series converges but each individual series does not.

$$V^N(R) = C(R) + \mathrm{IP}(R)\sum_{n=1}^{N-1} \mathrm{IP}^{n-1}(R)C(R) = C(R) + \mathrm{IP}(R)\sum_{\alpha=0}^{N-2} \mathrm{IP}^{\alpha}(R)C(R).$$

Therefore, $V^N(R) = C(R) + \mathrm{IP}(R)V^{N-1}(R)$.

$$V^N(R) = \sum_{n=0}^{N-1} \mathrm{IP}^n(R)C(R) =$$

$$\sum_{n=0}^{N-1}[\mathrm{IP}^n(R) - \tilde{I}\Pi(R)]C(R) + \sum_{n=N}^{\infty}[\mathrm{IP}^n(R) - \tilde{I}\Pi(R)]C(R) + N\tilde{I}\Pi(R)C(R) - \sum_{n=N}^{\infty}[\mathrm{IP}^n(R) - \tilde{I}\Pi(R)]C(R) =$$

$$V(R) + N\tilde{I}\Pi(R)C(R) + A_N(R)$$

where $\lim_{N\to\infty} A_N(R) = 0$.

$$V(R) + N\tilde{I}\Pi(R)C(R) = C(R) + \mathrm{IP}(R)[V(R) + (N-1)\tilde{I}|\Phi(R)C(R)] =$$

$$C(R) + \mathrm{IP}(R)V(R) + (N-1)\mathrm{IP}(R)\tilde{I}\Pi(R)C(R) = C(R) + \mathrm{IP}(R)V(R) + (N-1)\tilde{I}\Pi(R)C(R).$$

Note that $\mathrm{IP}(R)\tilde{I} = \tilde{I}$.

$$V(R) + \tilde{I}C(R) = C(R) + \mathrm{IP}(R)V(R),$$

$$V(R) + g(R)\tilde{I} = C(R) + \mathrm{IP}(R)V(R).$$

$$g(R)\tilde{I} = C(R) + [\mathrm{IP}(R) - I]V(R).$$

The unknowns are V(R) and g(R). We want to minimize g(R) and the long run costs of making decision R. Let $V_m(R) = 0$. Start with a policy R. Solve(*). This is called *value determination.* $0 < \alpha < 1$.

$$V^N(R) = \sum_{n=0}^{N-1} \alpha^n \mathrm{IP}^n(R)C(R) = C(R) + \alpha \mathrm{IP}(R)V^{N-1}(R),$$

$$V(R) = C(R) + \alpha \mathrm{IP}(R)V(R).$$

Using the generator example: $R_1(1) = 1, R_1(2) = 1, R_1(3) = 2, R_1(4) = 1$. Let $\alpha = 0.8 = \frac{4}{5}$. Then,

$$V_1(R_1) = 6 + \frac{4}{5}\left[\frac{3}{4}V_1(R_1) + \frac{1}{4}V_2(R_1)\right].$$

$$V_2(R_1) = 6 + \frac{4}{5}\left[\frac{1}{4}V_1(R_1) + \frac{3}{4}V_2(R_1)\right].$$

$$V_3(R_1) = 5 + \frac{4}{5}\left[\frac{3}{4}V_3(R_1) + \frac{1}{4}V_1(R_1)\right].$$

$$V_4(R_1) = 7 + \frac{4}{5}\left[\frac{3}{4}V_1(R_1) + \frac{3}{4}V_2(R_1)\right].$$

5.7.2 Homework

Problems 9,11,15,22,34.

5.7.3 Reliability

A system is made up of components $1, 2, 3, ..., n$, each of which works or fails. Let

$$x_i = \begin{cases} 1, & \text{if component } i \text{ works.} \\ 0, & \text{if component } i \text{ fails.} \end{cases}$$

The *system function* is

$$\phi(x_1, x_2, ..., x_n) = \begin{cases} 1, & \text{if component } i \text{ works.} \\ 0, & \text{if component } i \text{ fails.} \end{cases}$$

The *reliability* of the system is $R = P(\phi = 1) = E(\phi)$. A series function appears next.
$\psi(x_1, x_2, x_3, x_4) = x_1x_2x_3x_4$. A parallel function appears in Figure 5.32.

$\psi(x_1, x_2, x_3, x_4) = 1-(1-x_1)(1-x_2)(1-x_3)(1-x_4)$. The components are $1, 2, 3, ..., n$. What is the minimum components needed to keep the system working? This is called a *minimal path.* See Figure 5.33.

The paths are {1,3,5}, {2,4,5}, and {1,6,4,5}. Figure 5.34 is another example.

The paths are {1,5}, {1,3,6}, {2,4,6}. We must find all minimal paths. The system function is,

$$\Phi = \phi(x_1, x_2, x_3, x_4, x_5) = 1 - (1 - x_1x_5)(1 - x_1x_3x_6)(1 - x_2x_4x_6) =$$

$$1 - 1 + x_1x_5 + x_1x_3x_6 + x_2x_4x_6 - x_1x_3x_5x_6 - x_1x_2x_4x_5x_6 - x_1x_2x_3x_4x_6 + x_1x_2x_3x_4x_5x_6.$$

$$P(x_i = 1) = P_i.$$

$$R = P(\Phi = 1) = E(\Phi) = p_1p_5 + p_1p_3p_6 + p_2p_4p_6 - p_1p_3p_5p_6 - p_1p_2p_4p_5p_6 - p_1p_2p_2p_4p_6 + p_1p_2p_3p_4p_5p_6.$$

Example: Take the system diagram in Figure 5.34. The minimal paths are {1,5}, {1,3,6}, {2,4,6}.

$$\Phi(x_1, x_2, x_3, x_4, x_5, x_6) = 1 - (1 - x_1x_5)(1 - x_1x_3x_6)(1 - x_2x_4x_6).$$

Put bounds on the reliability. Let $x_1, x_2, ..., x_n$ be independent Bernoulli variables. Let $s_1, s_2, ..., s_k$ be subsets of {1,...,n} and for $j = 1, ..., k$, let $y_i = \Pi_{i\in s}x_i$.

$$s_1 = 2, 3, s_2 = 1, 3, 4, s_3 = 1, 4.$$

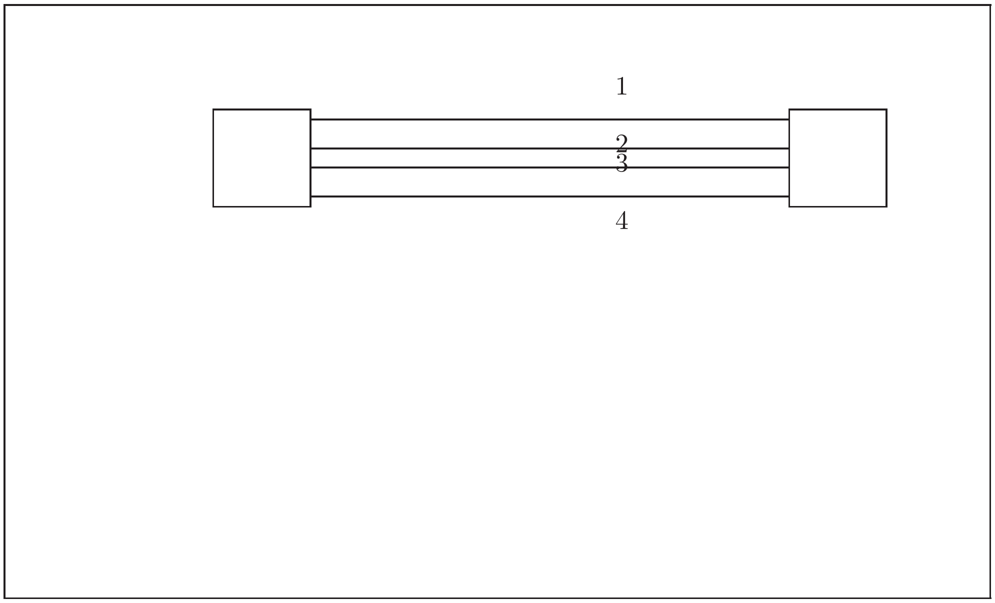


Figure 5.32: A Parallel Function

Create

$$y_1 = x_2x_3,\ y_2 = x_1x_3x_4,\ y_3 = x_1x_4.$$

$$P(y_1 = 0, y_2 = 0, y_3 = 0, ..., y_k = 0) \geq P(y_1 = 0)P(y_2 = 0)P(y_3 = 0)...P(y_k = 0).$$

Getting back to the example,

$$P(\Phi = 0) = P(x_1x_5 = 0, x_1x_3x_6 = 0, x_2x_4x_6 = 0) = 1 - R =$$

$$P(y_1 = 0, y_2 = 0, y_3 = 0) \geq P(x_1x_5 = 0)P(x_1x_3x_6 = 0)P(x_2x_4x_6 = 0).$$

$$s_1 = 1, 5, s_2 = 1, 3, 6, s_3 = 2, 4, 6.$$

$$P(x_1x_3x_6 = 0) = 1 - P(x_1x_3x_6 = 1) = 1 - p_1p_3p_6.$$

Therefore,

$$P(\Phi = 0) \leq (1-P(x_2x_5 = 1))(1-P(x_1x_3x_6 = 1))(1-P(x_2x_4x_6 = 1)) \leq (1-p_1p_5)(1-p_1p_3p_6)(1-p_2p_4p_6).$$

Therefore, $R \leq 1-(1-p_1p_5)(1-p_1p_3p_6)(1-p_2p_4p_6)$. Let $p_1 = 0.9, p_2 = 0.8, p_3 = 0.9, p_4 = 0.7, p_5 = 0.9, p_6 = 0.8$. Then $R = 0.9236$ or the upper bound is $R \leq 0.9634$. The *minimal cuts* in the last example are {5,6}, {1,2}, {1,4}, {3,4,5}, {2,3,5}, and {1,6}.

$$\Phi = [1 - (1 - x_1)(1 - x_2)][1 - (1 - x_5)(1 - x_6)]$$

$$[1 - (1 - x_1)(1 - x_4)][1 - (1 - x_3)(1 - x_4)(1 - x_5)]...$$

Next put bounds on the reliability using minimal cuts.

$$R = P((1 - x_5)(1 - x_6) = 0, (1 - x_1)(1 - x_2) = 0, ..., (1 - x_1)(1 - x_6) = 0).$$

$$R \geq P((1 - x_5)(1 - x_6) = 0)...P((1 - x_1)(1 - x_6) = 0).$$

Note the cuts give a lower bound and the minimal paths give an upper bound.

$$P((1 - x_5)(1 - x_6) = 0) = 1 - P(1 - x_5)(1 - x_6) = 1)$$

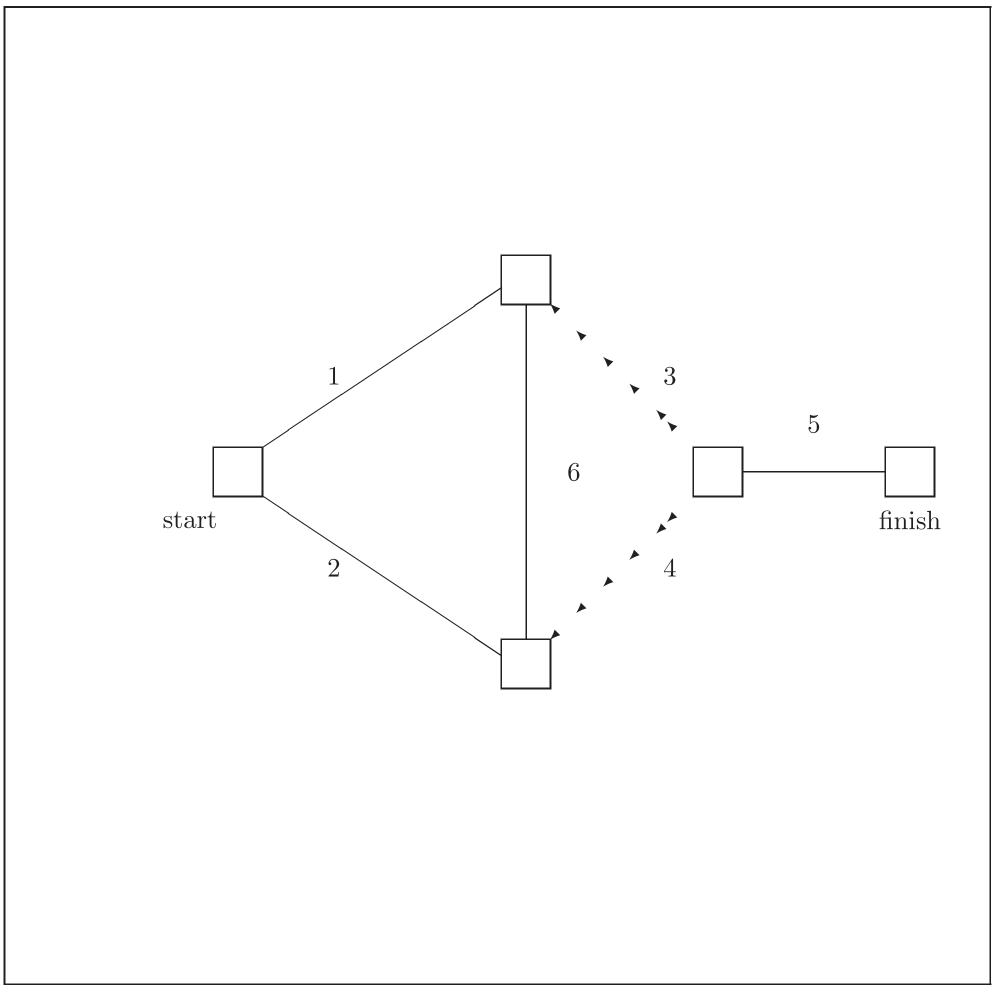


Figure 5.33:

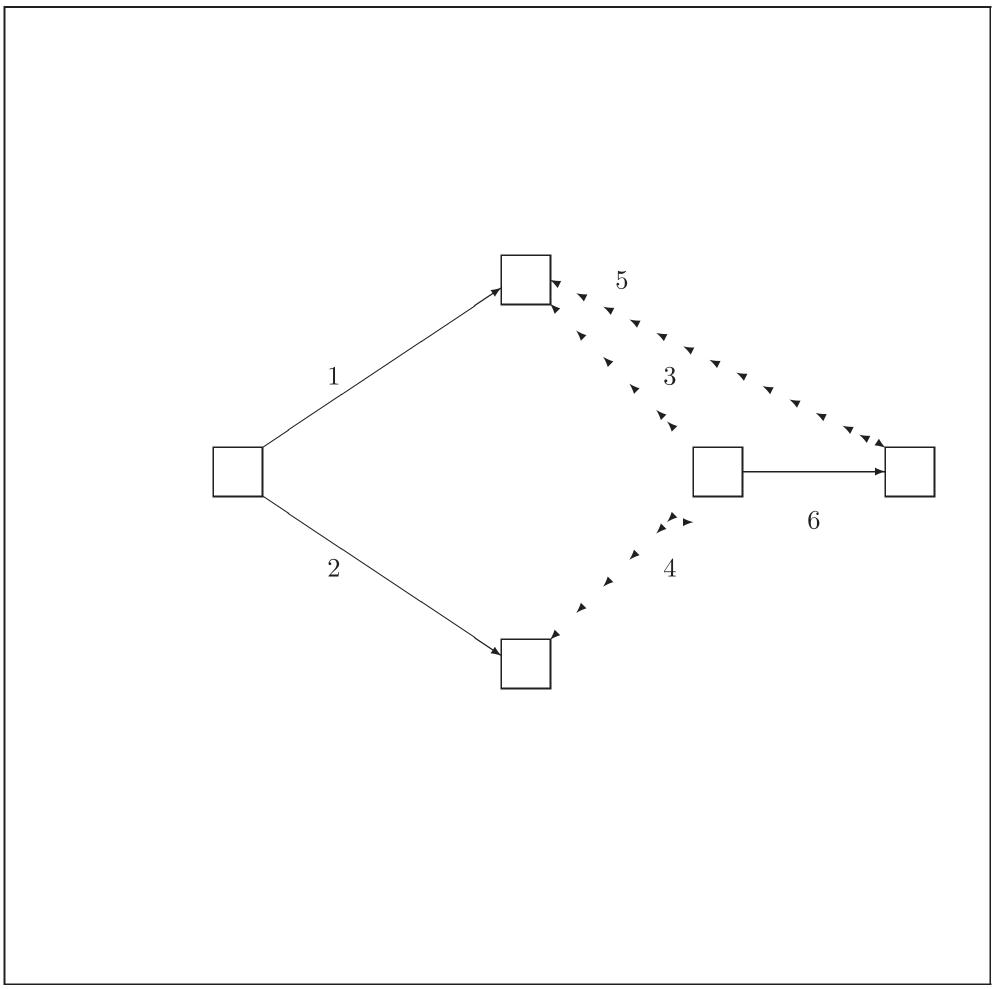


Figure 5.34:

.

.

.

$R \geq (1 - q_5 q_6)(1 - q_1 q_2)...(1 - q_1 q_6) = 0.9084.$

The true reliability is 0.9236.

5.7.4 Bayes Risk

Out of q_i possible actions, one must be chosen. Let Θ_j be the states of nature. There is a loss function $l(q_i, \Theta_j)$. Based on past experience, we have a *posterior* distribution $P(\Theta_j)$. $l(q_i) = \sum_j l(q_i, \Theta_j) P(\Theta_j)$. Choose $\min_j l(q_i)$.

Example: Build a cement plant in a region. The actions are build a large plant, build a small plant, and do not build a plant.

- $q_1 =$ build a large plant.
- $q_2 =$ build a small plant.
- $q_3 =$ do not build a plant.
- $\Theta_1 =$ higher sales.
- $\Theta_2 =$ moderate sales.
- $\Theta_3 =$ low sales.

The posterior distribution is $P(\Theta_1) = 0.1, P(\Theta_2) = 0.5, P(\Theta_3) = 0.4$. Let $l(q_i, \Theta_j)$ be

	Θ_1	Θ_2	Θ_3
q_1	-12	-4	2
q_2	-6	-5	1
q_3	0	0	0

$$l(q_1) = -12(0.1) - 4(0.5) + 2(0.4) = -2.4,\ l(q_2) = -2.7,\ l(q_3) = 0.$$

We can conclude to build a small plant since q_2 is the smallest. If an experiment can be done with possible outcomes w_k and $P(w_k|\Theta_j)$ are known, then *Bayes risk* for decision formation for Θ defined on $w_1, w_2, ...$ to $q_1, q_2, ...$

$$B(d) = \sum_j \sum_k l(d(w_k), \Theta_j) P(\Theta_j, w_k) = \sum_j \left[\sum_k l(d(w_k), \Theta_j) P(w_k|\Theta_j) \right] P(\Theta_j) =$$

$$\sum_j \sum_k \left[\sum_j l(d(w_k), \Theta) P(\Theta_j|w_k) \right] P(w_k).$$

Bayes formula is

$$P(\Theta_j|w_k) = \frac{P(\Theta_j, w_k)}{P(w_k)} = \frac{P(w_k|\Theta_j) P(\Theta_j)}{P(w_k)},$$

where

$$P(w_k, \Theta_1) + P(w_k, \Theta_2) + ...$$

Choose $d(w_k)$ to minimize $\sum_j l(\Theta(w_k), \Theta_j)P(\Theta_j|w_k)$.

Example: A *market* study can be made which will estimate future construction until the as w_1 high or w_2 low.

$$P_{w|\Theta} = \begin{array}{c|ccc} & \Theta_1 & \Theta_2 & \Theta_3 \\ \hline w_1 & 0.8 & 0.5 & 0.3 \\ w_2 & 0.2 & 0.5 & 0.7 \end{array}$$

$$P(w_1) = \sum_j P(w_1|\Theta_j)P(\Theta_j) = (0.8)(0.1) + (0.5)(0.5) + (0.3)(0.4) = 0.45.$$

$$P(w_2) = 0.55.$$

So,

$$P_{\Theta|w} = \begin{array}{c|ccc} & \Theta_1 & \Theta_2 & \Theta_3 \\ \hline w_1 & 0.1778 & 0.5556 & 0.2667 \\ w_2 & 0.0364 & 0.4545 & 0.5091 \end{array}$$

$$P(w_1, \Theta_1) = \frac{P(w_1|\Theta_1)P(\Theta_1)}{P(w_1)} = \frac{(0.8)(0.1)}{0.45} = -0.1778.$$

$$l(q_1) = \sum_{j=1}^{3} l(q_1, \Theta_j)P(\Theta_j|w_1) = (-12)(0.1778) + (-4)(0.5556) + (2)(0.2667) = -3.8226.$$

$$l(a) = \begin{array}{c|ccc} & q_1 & q_2 & q_3 \\ \hline w_1 & \text{-3.8226} & \text{-3.5781} & 0 \\ w_2 & \text{-1.2366} & \text{-1.9818} & 0 \end{array}$$

Therefore, $d(w_1) = q_1$ and $d(w_2) = q_2$.

$$B(\Theta) = \sum_j l(q_1, \theta_j)P(\Theta_j|w_1)P(w_1) + \sum l(q_2, \Theta_j)P(\Theta_j|w_2)P(w_2) =$$

$$((-3.8226)(0.45) - 1.9818)(0.55) = -2.8102.$$

That is the expected loss with the study. Therefore, the maximum to pay for the study is 2.8102-2.7=0.1102. The amount to pay for perfect information is (-12)(0.1)+(-5)(0.5)+0(0.4) = -3.7. The most money you should be willing to pay for a study is 1.0(3.7 - 2.7). Alternately, the last example can be organized into a decision tree. E(cost node 1)=(0.1)(-12)+(0.5)(-4)+(0.4)(2). E(cost node 2)=(0.1)(-6)+(0.5)(-5)+(0.4)(1). E(cost node 3)=0.

Chapter 6

Network Optimization

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Math 576, Spring 1993

Text used: Phillips and Garcia-Diaz *Fundamentals of Network Analysis* Waveland Press, Inc, Prospect Heights, IL 1990

6.1 Network Representation

How can we represent a network in a computer?

1. Adjacency matrix. In an adjacency matrix, $a_{ij} = 1$ if vertices i and j are connected directly by an edge (i, j). a_{ij} is zero otherwise. An undirected network is symmetric matrix-wise.

2. Node-arc incident matrix. Let N be a matrix with m rows(nodes), one for each vertex, and n columns, one for each edge. Then, if n_{ij} is the element in the i-th row and j-th column, let $n_{ij} = 1$ if edge j is incident with vertex i, zero otherwise, -1 if directed into j.

   Example: See Figure 6.1. The node-arc matrix is given by:

$$\begin{array}{c|ccccc|} & \text{a} & \text{b} & \text{c} & \text{d} & \text{e} \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 2 & -1 & 1 & 0 & 0 & 1 \\ 3 & 0 & -1 & -1 & 1 & 0 \\ 4 & 0 & 0 & 0 & -1 & -1 \end{array}$$

   For all network problems, except for upper or lower bound constraints, each column has exactly two non-zeros in the constraint matrix, one of which is $+1$ while the other is -1.

3. Distance matrix.

6.2 Network Terminology

Example: The Kongsberg Bridge Problem. The problem was first presented by Euler. See Figure 6.2
The question is, can you cross each bridge once and get back home? No. Make each land mass a node and each bridge an arc. This problem cannot be solved due to the degree of the nodes. There is an odd number of arcs. It only works when all degrees are even. Points on the graph are called *vertices* or *nodes* denoted by

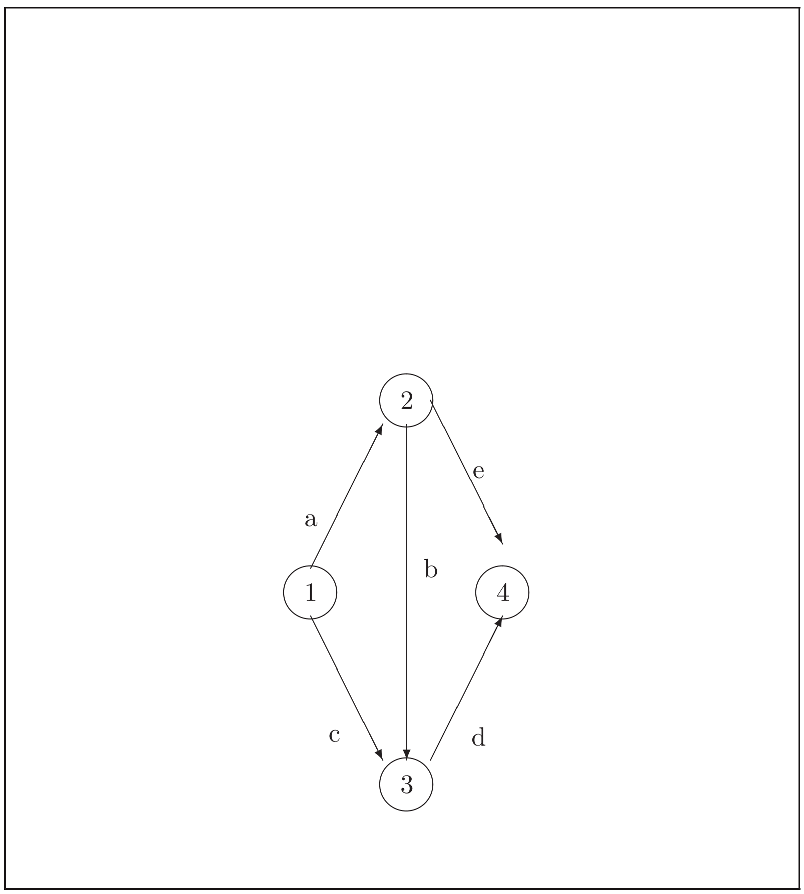

Figure 6.1: A Directed Graph

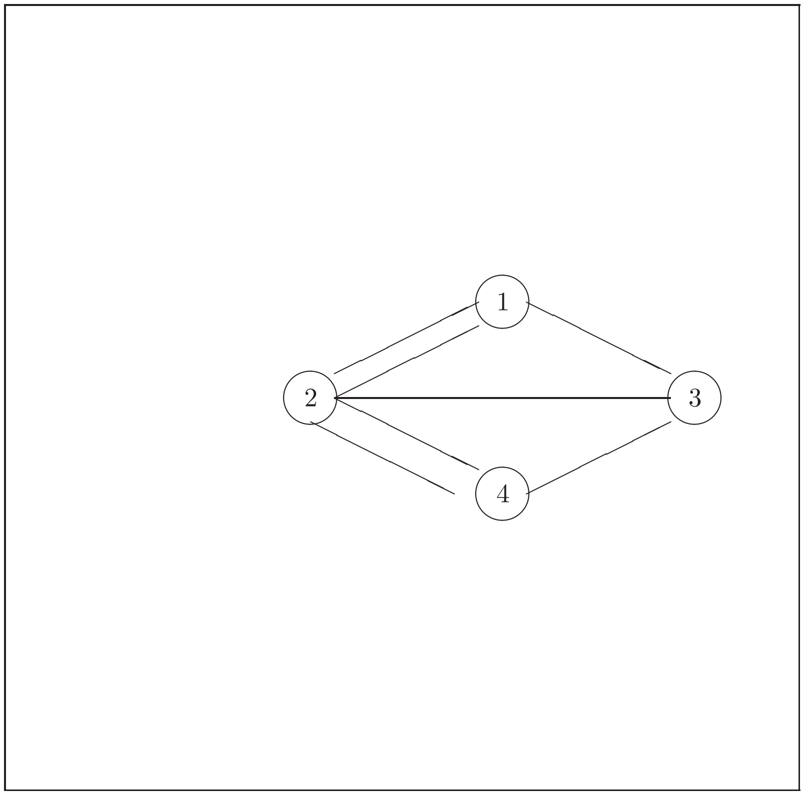

Figure 6.2: Kongsberg Bridge Problem

$(1, 2, ..., n)$. Connecting lines are *arcs* or *edges* denoted by $(a, b, c, ...)$. A *graph* is a collection of vertices and edges. So, $e_1 = (1, 2)$, $e_2 = (1, 2)$, $e_3 = (2, 3)$, $e_4 = (1, 3)$, etc. A graph G is a set of x whose elements are nodes and a set E of edges, G(x,E). Nodes can represent time. The beginning node is the *head.* The ending node is the *tail.* A graph with one or more numbers associated with each arc is a *network.* c_{ij} is the cost of traversing an edge from node i to node j. A *loop* is a node that points to itself.

For a loop-less graph with no multiple edges, if $|x| = m$ and $|E| = n$, then $n \leq \frac{m(m-1)}{2}$. Any graph where every pair of nodes is connected by an edge is called a *complete graph.* The degree must be $n - 1$ for every node. A graph is *planar* if it can be drawn with no two edges crossing each other. An *incident vertex and edge* is when the edge comes out of the vertex. Two edges are *adjacent* if incident to the same node. A *path* is any sequence of edges that can be followed. *Length of path* is the number of edges in the path. A *cycle* is when a path has a node as the initial node and as the terminal node. A *tree* of a graph is when a graph is connected and the graph contains no cycles. A *forest* is any graph that contains no cycles. It is a collection of trees. A *spanning tree* is when a subgraph touches every node in the graph.

6.3 Shortest Route Problems

The *shortest route problem* is given a collection of nodes and arcs, with a set of positive arc parameters c_{ij}, find the path from the source node s to the sink node t that minimizes the cost of shipping one unit of flow from the source to the sink.

Example: Consider the problem of processing over 137,700,000 questionnaires. Four CPM models were developed where the nodes represent activities in a given warehouse and the arcs represent hours to complete those activities *for one day.* The longest path through the network was 1,536 hours.

Example: Finite planning horizon models. Let the nodes be time periods in which a machine is replaced. Let the cost c_{ij} of buying a new machine be an arc. Find the shortest route that minimizes costs.

Example: Activity on node model. Let the nodes be tasks in a project. Let the arcs be durations of time d_i in which a task is completed. Use a dummy node for the start and finish. The longest chain from start to finish represents the *minimum project duration.*

Example: Activity on arc model. Let the arcs be tasks and use dummy nodes. As an example, building a building.

In the CPM(critical path method), the longest chain in a model is called the *critical path.* A delay in any task will result in a delay in project completion. PERT(program evaluation and review technique) provides an estimate of mean project completion and variance.

Example: Scheduling tanker voyages. Let a network be scheduling ports to visit. Each node is a port. Each arc has a cost c_{ij} and a transit time t_{ij}. find the maximum average profit per time unit by minimizing

$$\frac{\sum c_{ij}}{\sum t_{ij}}.$$

Distance networks are used to ship one unit of flow through the nodes in a network. The arcs are distances with a generalized cost of using the arc. *Capacitate flow networks* include a *capacity* or a maximum amount of flow per unit of time that can be shipped along an arc. Let f_{ij} be the flow of an arc. Then,

1. Maximize the value of flow, v.
2. $$\sum_j f_{ij} - \sum_j f_{ji} = \begin{cases} v, & i = 1. \\ 0, & i \neq 1, i \neq n. \\ -v, & i = n. \end{cases}$$
3. $0 \leq f_{ij} \leq u_{ij}, (i,j) \in E.$

Additional parameters: Let c_{ij} be a cost coefficient for each arc (i,j) with an upper and lower bound u_{ij} and l_{ij}. b_i is the supply. $b_i \geq 0$ is the source, $b_i = 0$ is an intermediate node and $b_i < 0$ is the terminal node. Then, we want to

1. Minimize $\sum_i \sum_j c_{ij} f_{ij}$.
2. $\sum_j f_{ij} - \sum_i f_{ji} = b_i, i \in N.$
3. $l_{ij} \leq f_{ij} \leq u_{ij}, (i,j) \in E.$

In *transportation problems,* suppose m is the number of plants and n is the number of warehouses. Each plant has a supply $s_i, i = 1, 2, ..., m$. Each warehouse creates a demand $d_j, j = 1, 2, ..., n$. Minimize the total shipping costs. That is minimize $\sum_i \sum_j c_{ij} x_{ij}$ subject to:

1. $\sum_j x_{ij} = s_i, i = 1, 2, ..., m.$
2. $\sum_i x_{ij} = d_j, j = 1, 2, ..., n.$

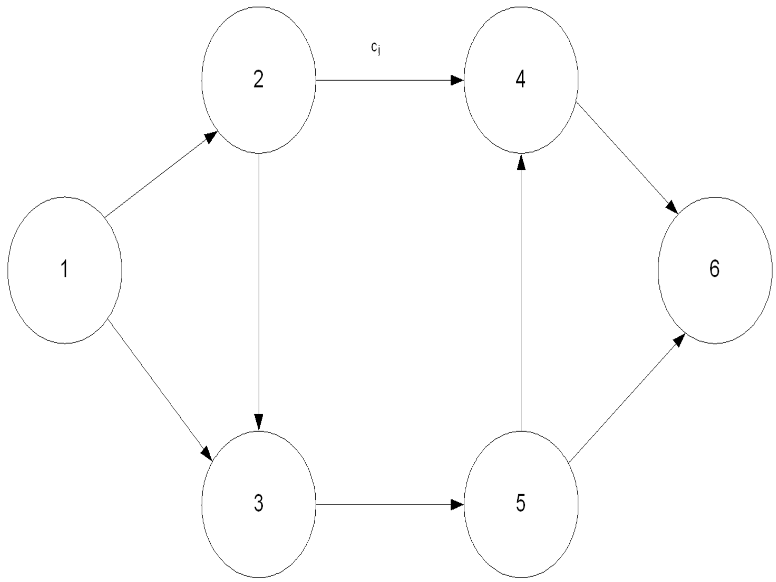

Figure 6.3: Trucks entering a state government example.

3. $x_{ij} \geq 0, i = 1, 2, ..., m; j = 1, 2, ..., n$.

Example: Trucks that enter a state must file a road plan with the state government. See Figure 6.3. Some roads are congested and slow, some dangerous, some prohibited to truck over a certain size. c_{ij} can be the cost of traversing a arc (i, j). The cost can be mileage, time, congestion, insurance premium, or a danger measure. m is the cost of an impossible arc.

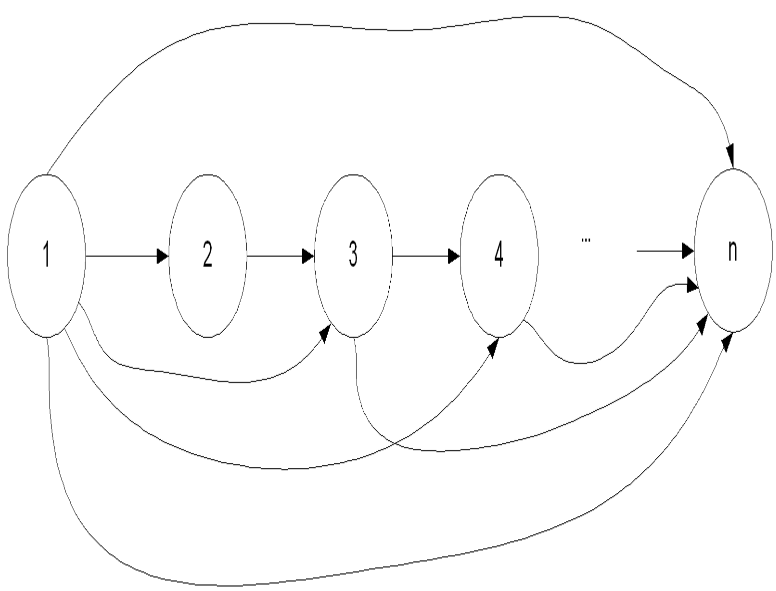

Figure 6.4: The equipment replacement problem example.

Example: An equipment replacement problem. See Figure 6.4. The nodes are time. The arcs are the different strategies. c_{ij} is the cost of equipment. In each time period, you have a choice 1) keep the equipment, or 2) buy new equipment. If you buy in period i and sell in $j-1$, the cost $i-j$ is c_{ij} the acquisition cost in i plus the total maintenance costs from i thru $j-1$.

Example: Salesperson routing. A sales person travels from Boston to LA on the interstate highway system. You can visit other clients on the way and earn commissions. We want to minimize the cost of the total trip cost. The trip cost is travel cost minus commissions. Note: Commissions could exceed travel cost. Thus, Dijkstra's algorithm cannot be used.

Example: Investment planning. How to invest funds in coming years. Assume for simplicity that investments can be made on the first of each month into CD's, stocks, bonds, etc. See Figure 6.5.

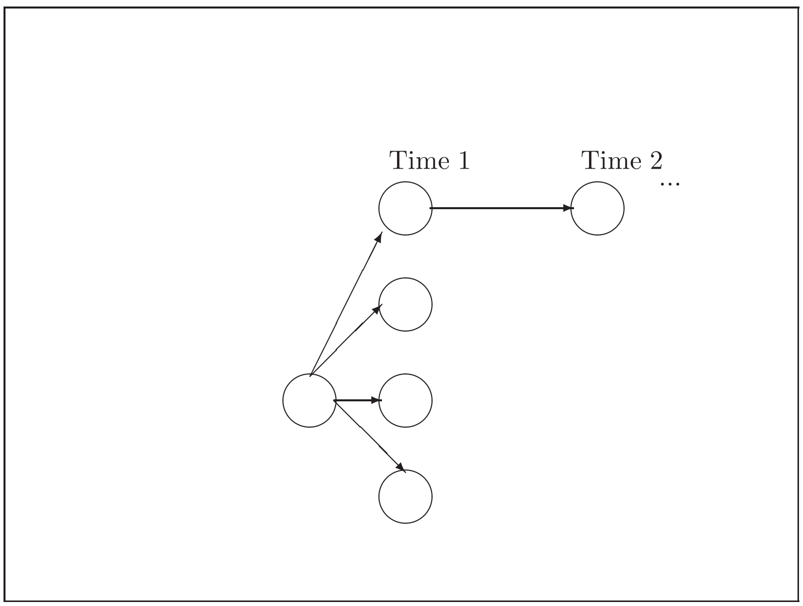

Figure 6.5: Investments

Note that flow in does not equal to flow out. The problem is to find the longest route.

Example: Production lot size problem. See Figure 6.6. Determine a schedule of production runs when the demand varies deterministically over time. Demands D_1, D_2, ..., D_n are given over an n period of time. In each period where we produce at all, we incur a fixed cost A_j as well as a unit production cost c_j. Any amount left over in a period after demand is met is held in inventory until the next period, increasing a per unit holding cost of H_j. This problem can be formulated as a shortest route problem, similar to equipment replacement. How can we draw the graph? Let the nodes be time periods.

6.3.1 Dijkstra's Algorithm

A ratio edit requires that the ratio of two data items is bounded by lower and upper bounds (of the form $l_{ij} \leq \frac{v_i}{v_j} \leq u_{ij}$, where l_{ij} and u_{ij} are the lower and upper bounds respectively). Any pair of ratio edits that contain a common data item implies another ratio edit. The modified Dijkstra algorithm can been used to find the complete set of edits.

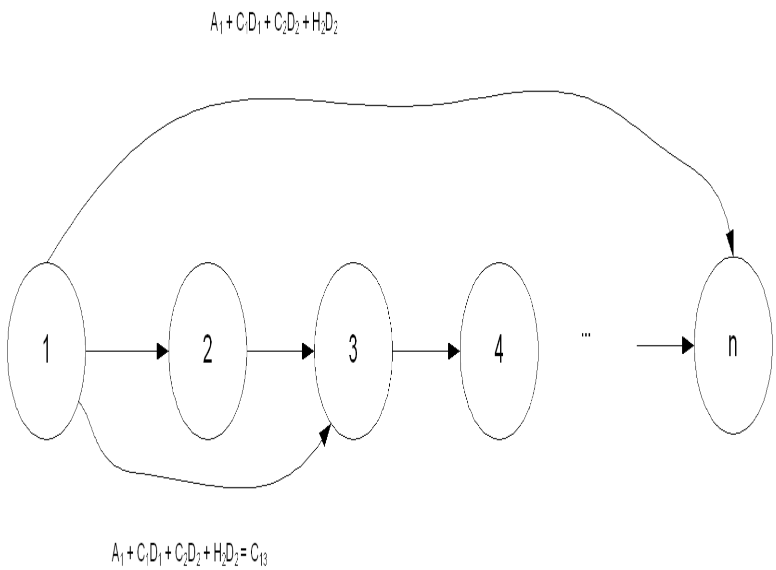

Figure 6.6: The production lot size example.

All arcs must be non-negative. A *label* is made permanent at each iteration. n iterations are required for n nodes. The main idea: Suppose we know k vertices that are closest to s vertex and also the shortest path from s to each of these vertices. Label vertex s and these k vertices with their shortest distances from s. Then, the $(k+1)$-st closest vertex to x is found as follow: for each labeled vertex, construct k distinct paths from s to y by joining the shortest path from s to x. Select the shortest of these and make it permanent.

Example: Dijkstra's Algorithm. See Figure 6.7.

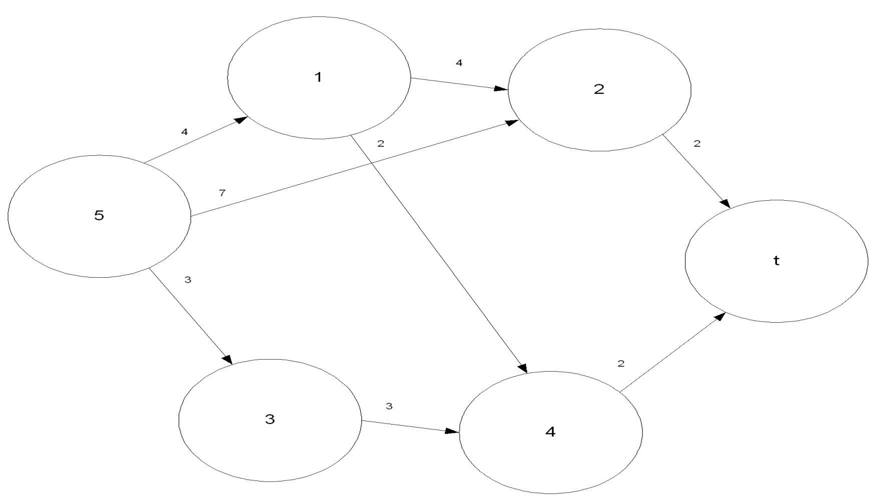

Figure 6.7: *Dijkstra's algorithm example.*

Step 1: $d(s) = 0$, $d(i) = \infty$ for all others.

Step 2:

$$d(1) = \min(d(1), d(s) + a(s, 1)) = \min(\infty, 0 + 4) = 4.$$

$d(2) = \min(\infty, 7) = 7.$

$d(3) = \min(\infty, 3) = 3.$

Choose the minimum of these and make it permanent. The minimum is $d(3) = 3$.

$$d(4) = \min(d(4), d(3) + a(3,4)) = \min(\infty, 3+3) = 6.$$

Make $d(1) = 4$ permanent, etc. Then, the tree would be s–3, s–1, s–3–4, s–2, s–3–4–t.

For the solution, see Figure 6.8 and Figure 6.9. Note that the two graphs are the same and are correct.

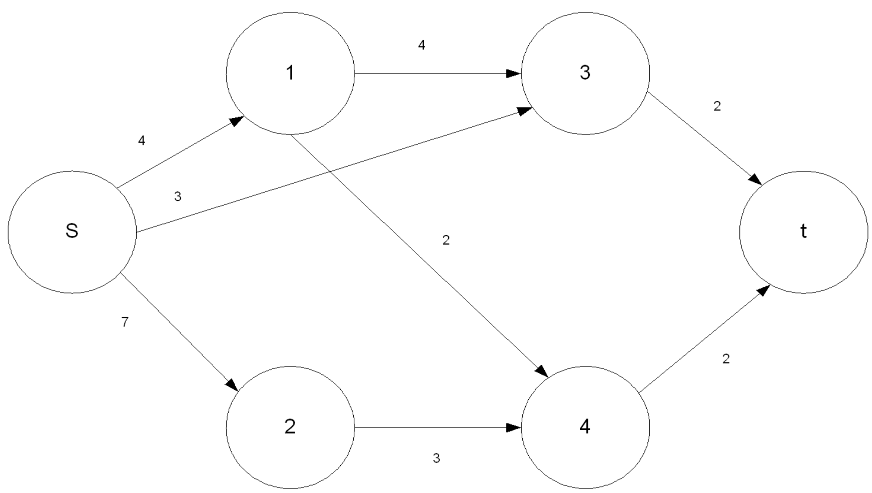

Figure 6.8: *This figure shows the results of applying Dijkstra's algorithm.*

6.3.2 Dynamic Programming

Dynamic programming can be used to solve shortest route problems. It requires directed arcs, no cycles, and all costs must be non-negative. The name dynamic refers to time. This procedure solves the problem backwards. For example, take the graph is Figure 6.7. Start at t and goto nodes 2 and 4. The minimum between nodes 2 and 4 would be chosen. See Figure 6.11.
The advantage of dynamic programming is that the algorithm is simple and there are no temporary labels as in Dijkstra's algorithm. The disadvantage of dynamic programming is that Dijkstra's algorithm works on more problems. See Figure 6.12.

Section 2.5 of the text book has shortest path models with fixed charges. Additional penalties or costs are associated with traversing one or more nodes. Examples include port costs, transshipment time delays, rental costs for storage facilities, etc.

Example: The number m(red) is the number associated with visiting the node. Arc costs are travel costs. How would you solve it? See Figure 6.13.
Node costs are hotel and meal costs at city i, arc costs are gas, oil, tolls, and time costs. How could you create a new network whose shortest route minimized the total costs?

Example: Similar idea in the text book. Turn penalties on page 69. Each turn costs 3 units. See Figure 6.14.
Theorem: In a network with turn penalties, the shortest path from node s to node t thru an intermediate node k may not include the shortest route from s to k or from k to t.

Step 1: Add a source node and a terminal node.

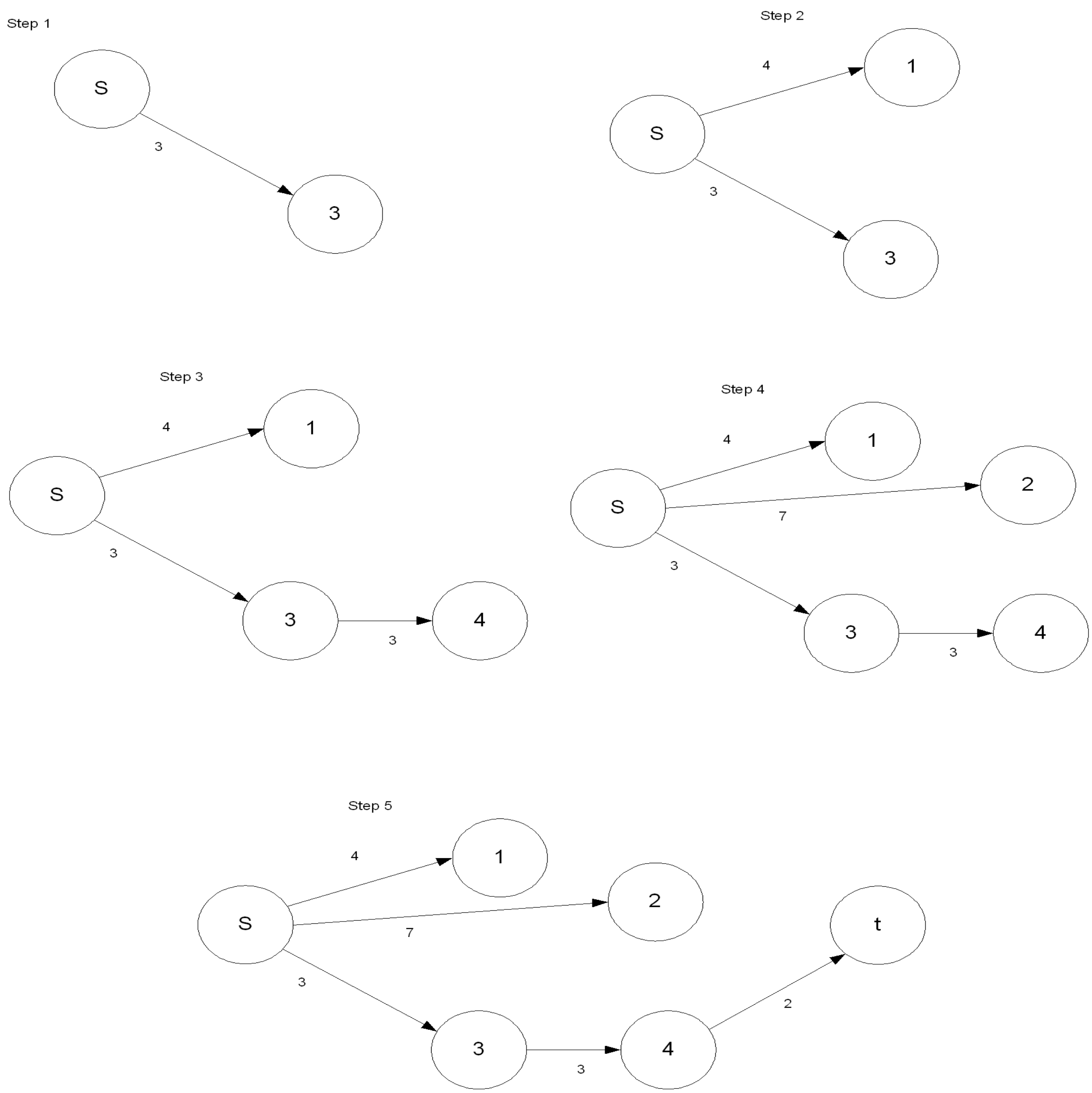

Figure 6.9: *This figure shows the individual steps of applying Dijkstra's algorithm.*

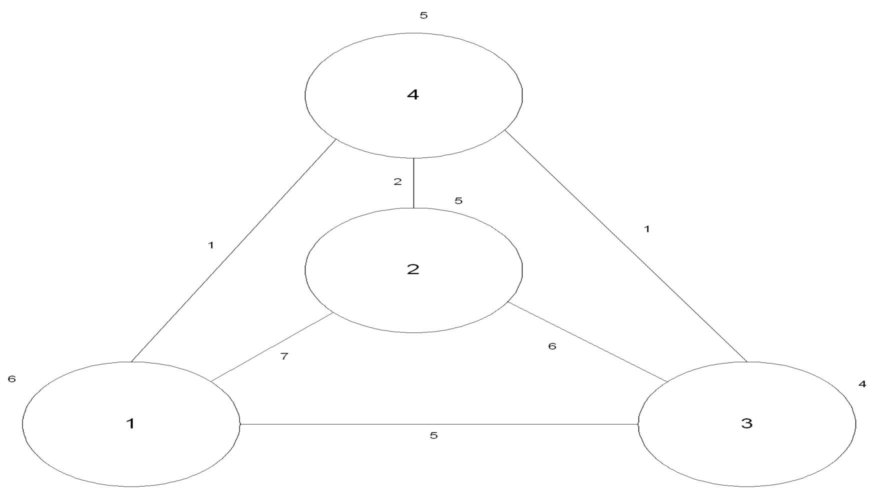

Figure 6.10: *This figure shows the site selection graph.*

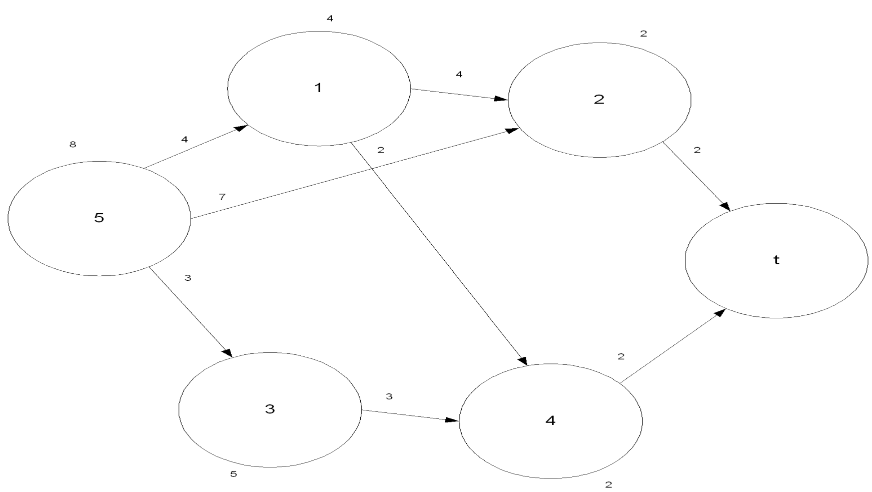

Figure 6.11: *Solving the shortest route problem using dynamic programming.*

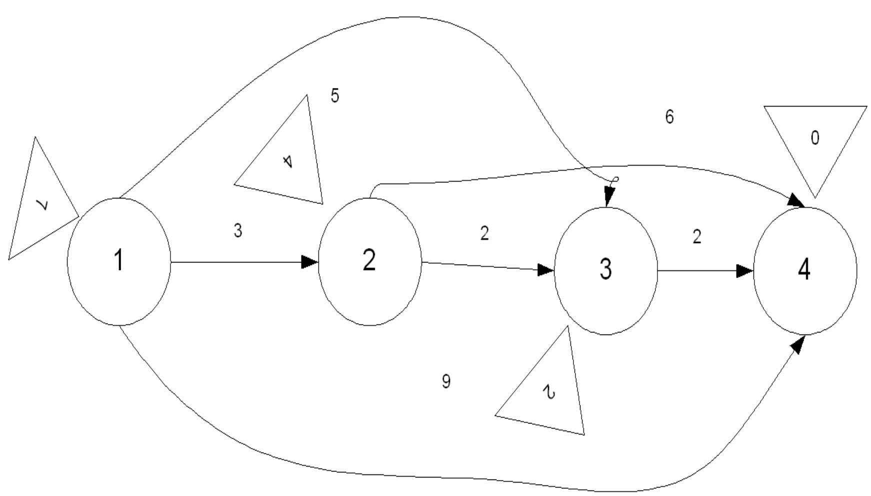

Figure 6.12: *Equipment replacement example.*

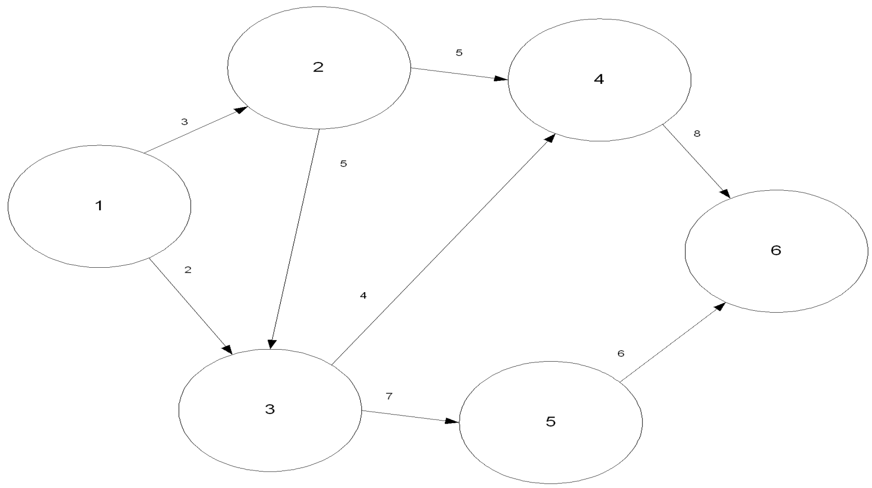

Figure 6.13: *Node costs are hotel and meal costs.*

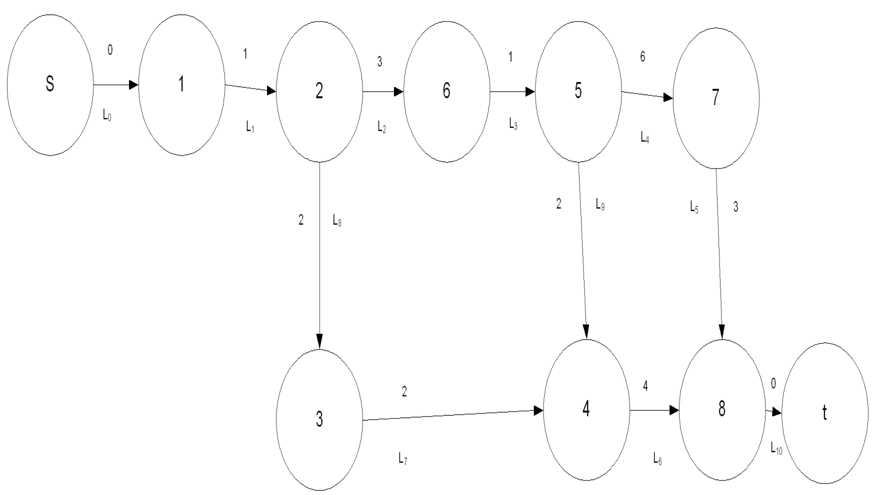

Figure 6.14: *Turn penalty problem.*

Step 2: Label each arc $L_0, L_1, ..., L_{10}$ as shown. The numbering is arbitrary.

Step 3: Create a pseudo-network with $L_0, L_1, ..., L_{10}$ as nodes. (L_i, L_j) has arc cost $C(L_i)+p(L_i, L_j)$ where $C(L_i)$ is the original cost of L_i from step 2 and where $p(L_i, L_j)$ is the turn penalty(0 or 3) associated with the branch (L_i, L_j).

Example: Arc costs. (L_1, L_8) has a cost of $4 = 1 + 3$. (L_1, L_2) has a cost of $1 = 1 + 0$. The new network with these pseudo costs can be solved by Dijkstra's algorithm. See Figure 6.15.

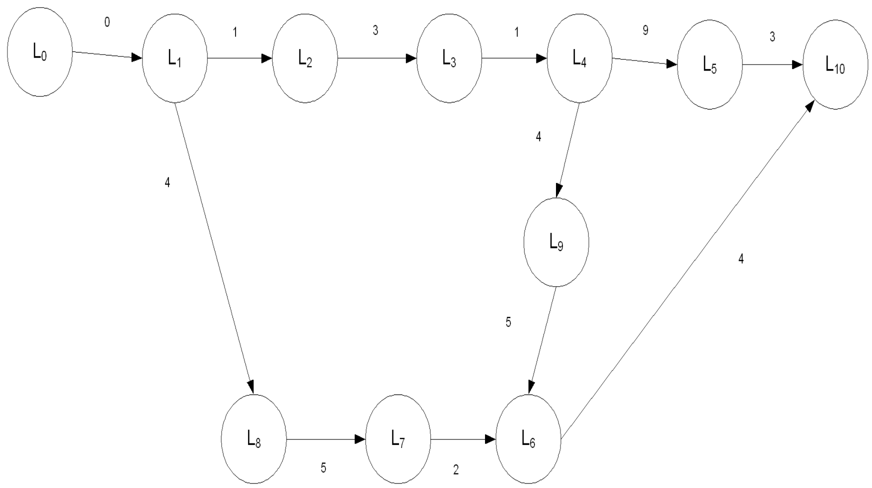

Figure 6.15: *The new network with pseudo costs.*

The optimal solution is $L_0, L_1, L_8, L_7, L_6, L_{10}$.

Instead of merely finding the single shortest route from s to t, find $2, 3, ..., k$ shortest routes. Why bother? Reliability, congestion, capacity.

The algorithm called *double sweep* finds the k shortest paths from s to other nodes. It was developed by Doug Shier. Very complex!

6.3.3 Algorithmic Complexity

Algorithms are increasingly important in solving OR problems iteratively. Effective algorithms solve problems easily, e.g. MST. Dijkstra's is effective too. As the problem gets larger, the algorithm remains efficient. On shortest route problems, there is an answer at each iteration. Enumeration is terrible.

6.3.4 Minimal Spanning Trees

Example: Cable service must connect 6 housing developments so that there is a path from each node to every other node. There is a cost associated with each potential arc (i, j). Find the set of arcs which connects the nodes at a minimum cost. See Figure 6.16.

Is this problem easy to solve mathematically? Yes. Is this problem easy to formulate as an LP?

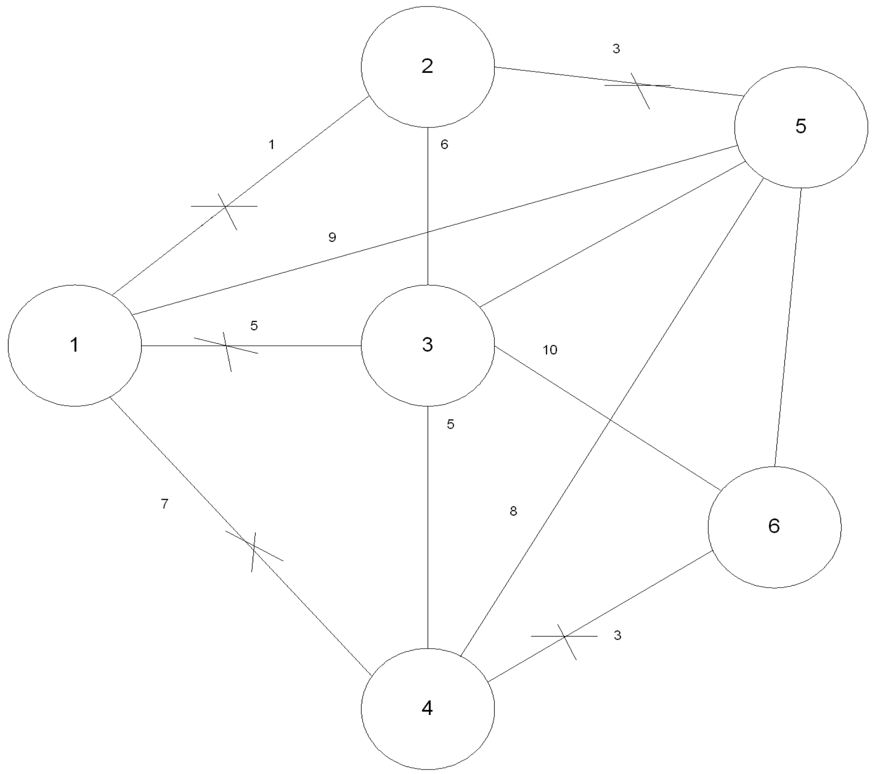

Figure 6.16: Housing Developments

Example: Rumor monger. Each villager is a node. Each may tell 0, 1, or many others. Each must be told once and there has to be a path from the originator to the villager.

Example: Highway construction. See Figure 6.17.

The costs in this example are:

	1	2	3	4	5
1	–	5	50	80	90
2	5	–	70	60	50
3	50	70	–	8	20
4	80	60	8	–	10
5	90	50	20	10	–

6.3.5 Shortest Path Problems as Transshipment Problems

Minimize the cost of sending 1 unit from node 1 to node n. All other points are transshipment points. Cost of arc (i, j) is the length of (i, j) if an arc exists, m otherwise. Cost of arc (i, i) is zero.

Example: See Figure 6.18.

Go from node 1 to node 7 at the minimal cost.

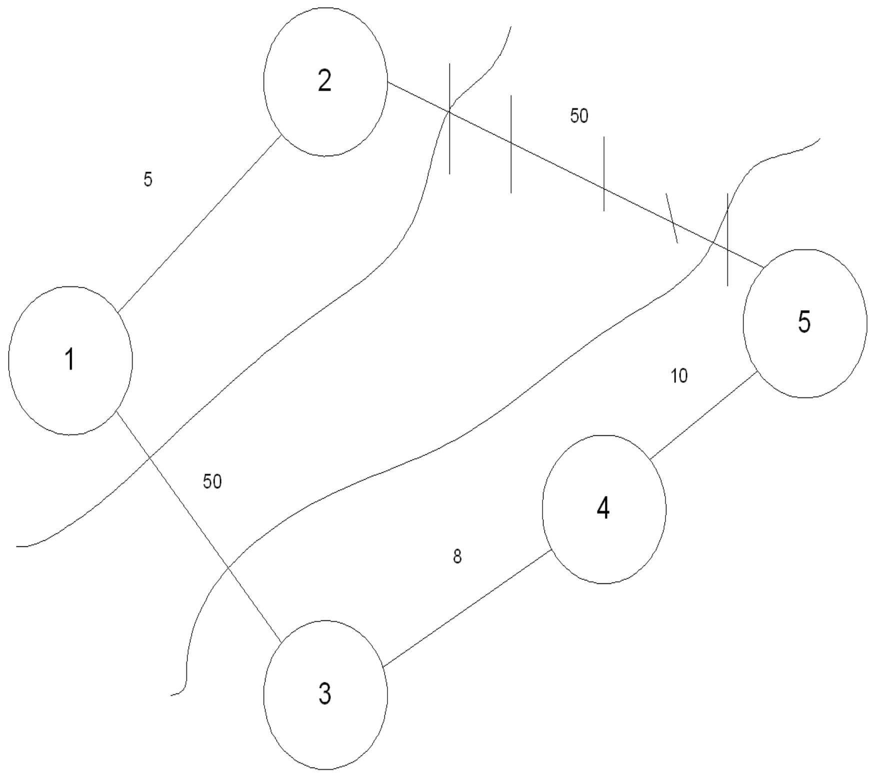

Figure 6.17: The highway construction example.

	1	2	3	4	5	6	7
1	(2)	1(2)	(8)	(11)	(9)	(m)	(m)
2		(0)	(3)	(m)	(5)	1(1)	(m)
3		(4)	1(0)			(2)	
4			(9)	1(0)		(2)	(23)
5					1(0)	(7)	(9)
6		(8)	(3)	(5)	(1)	(0)	(10)

Solve to get the solution, $x_{12} = 1$, $x_{26} = 1$, $x_{33} = 1$, $x_{44} = 1$, $x_{55} = 1$, $x_{67} = 1$. The optimal route is 1–2–6–7 and the minimal cost is 13.

6.3.6 Shortest Route as an LP

Rules:

1. Each variable corresponds to an arc.
2. Each constraint corresponds to a node.
3. x_{ij} is the amount of flow in (i, j), or $(0, 1)$.

The general formulation for finding the shortest route from 1 to n :

$$\min(z) = \sum_{(i,j)} \sum c_{ij} d_{ij} x_{ij}$$

subject to the following constraints:

$$\sum_{(i,j)} x_{ij} = 1, \text{for the source node.}$$

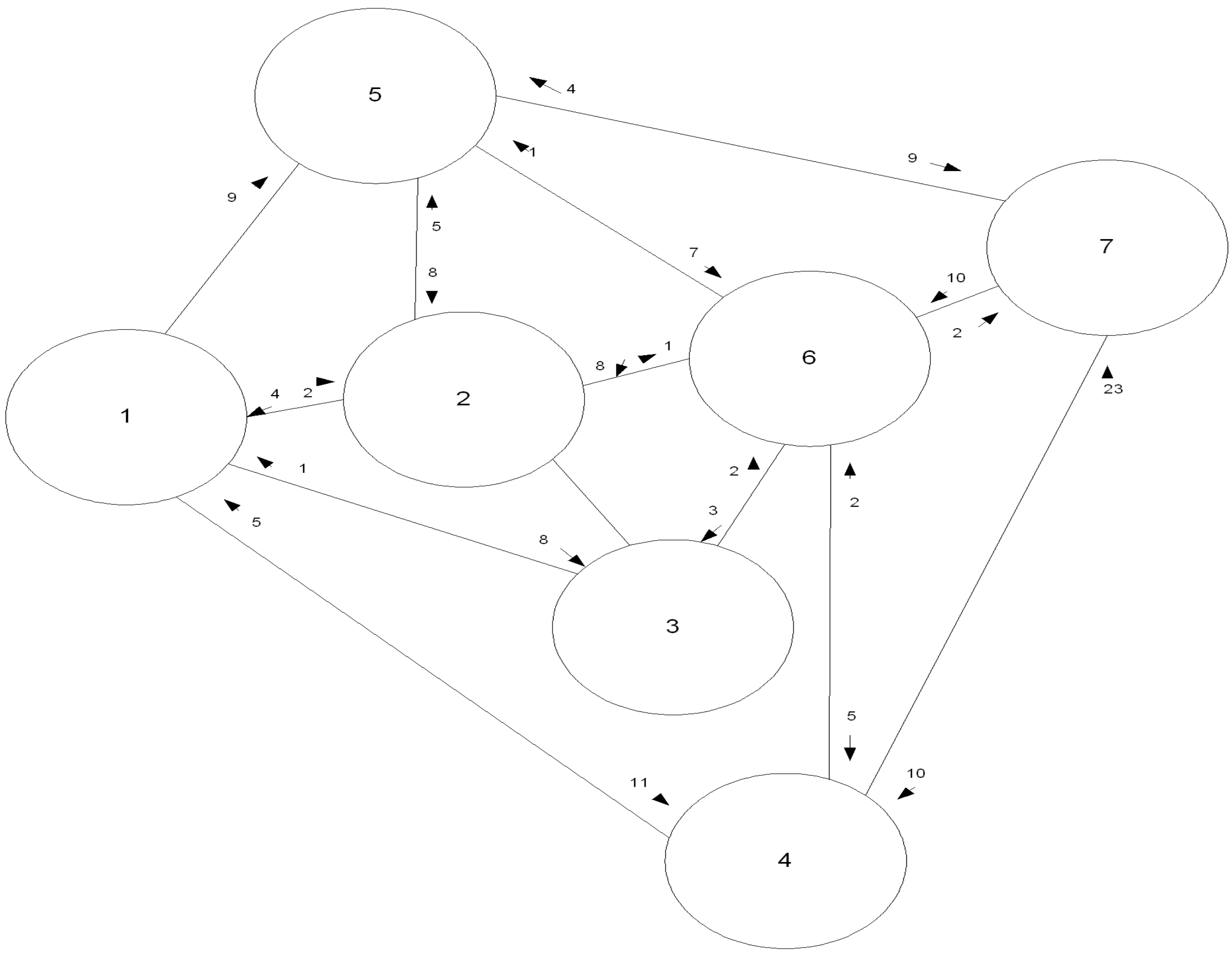

Figure 6.18: *Transshipment Network*

$$\sum_{(i,k)} x_{ik} = \sum_{(k,j)} x_{kj} \forall k \neq 1, n.$$

$$\sum_{(i,n)} x_{in} = 1,$$

and $x_{ij} \geq 0, \forall i, j$.
Try now to formulate the problem as a math programming problem. Assume $D = \{d_{ij}\}$ is asymmetric. We wish to minimize $\sum_i \sum_j d_{ij} x_{ij}$ subject to $\sum_i x_{ij} = 1, \forall j$, and $\sum_j x_{ij} = 1, \forall i$. Respectively, it means only cut j has to have one arch coming into it, and city i has to have one arc coming out of it. The last condition is $\sum_{i \in S} \sum_{j \in X-S} x_{ij} \geq 1, \forall S \subseteq X$. We need a third constraint that satisfies 1 and 2 and obviously this is not enough. We need more constraints to force a single cycle. For example, $X = \{1, 2, 3, 4\}$. $S = \{1\}, \{2\}, ...\{4\}, \{1, 2\}, ..., \{3, 4\}, ..., \{1, 2, 3\}, ...\{1, 3, 4\}, ..., \{1, 2, 3, 4\}$. So, you see a lot of subsets for $n = 4$. $S - X$ is the compliment.

The LP is not used often for the traveling salesman problem because it is too long with too many constraints.

Example: Choose $\{S\} = \{1\}$. Then, $X - S = \{2, 3, 4\}$. Then, $x_{12} + x_{13} + x_{14} \geq 1$. At least one (if not more) arcs connecting these points.

Example: $S = \{1, 2\}$. $X - S = \{3, 4\}$. $x_{13} + x_{14} + x_{23} + x_{24} \geq 1$. Often they will set the problem up to force a computer program to formulate the added constraints.

Symmetric Traveling Salesman Problem

If the problem is symmetric, then $i \to j$ and $j \to i$ then just change the notation for the number of arcs. $\min \sum_t d_t x_t$ subject to $\sum x_t = n$, $x_t = 0, 1$, t is the number of arcs, $\sum_{t \in (S,t)} x_t \geq 1, \forall (S, t), S \subseteq X$, $\sum_{t \in A_i} x_t = z, \forall i = 1, 2, ..., n$ where A_i is the set of arcs connected to node i.

Traveling Salesman Problem

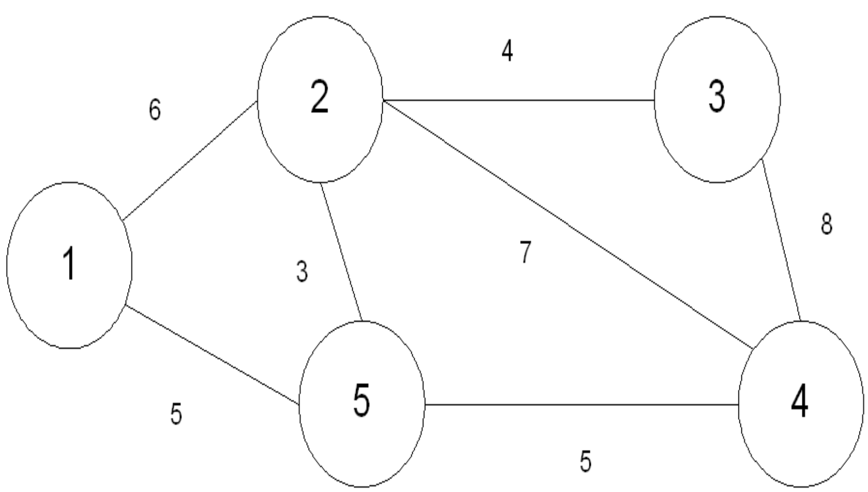

Figure 6.19: An example of a maximum capacity route.

We need a cycle that includes each vertex in G exactly once. This is called a *Hamiltonian cycle.* We want one with the smallest length, and get the upper and lower bound. The upper bound provides a feasible solution. It may not be optimal, though. The lower bound, if it is feasible, certainly is optimal, but usually not feasible. If the interval of the lower-to-upper bounds is small enough, you can choose the upper bound which is feasible and have a heuristically good solution.

Example: Collection and Delivery problem. Examples include: Fed-X, UPS, Postal Service, etc. How should trucks be routed? Urban services such as garbage collection, school buses, etc are included. Traveling requires a repairer or vendor. In what order should sites be visited?

Example: Ice cream flavor schedule. You have to make your own ice cream. Suppose that you had a lot of flavors to make. What is the best order?

Example: Suppose the highways are allocated to have junctions at places other than the five towns.

Example: Maximum capacity rate. Given an undirected network in which each edge (x, y) has a capacity $C(x, y)$ that represents the max amount of flow that can pass through (x, y).

The maximum weight spanning tree problem solves the max capacity rate problem. See Figure 6.19. The numbers in the graph represent capacities, not costs. An example would be rush hour traffic and highways. We would want to study the max capacity.

Facility Layout

We wish to arrange m facilities (i.e. different departments in a library). A traffic study results in a matrix specifying the number of trips made at each pair of facilities.

Example: The library example. We would put the rare books room in the back basement, but we would not put circulation there. Consider the following matrix.

		1	2	3	4	5
Entrance	1	–	–	–	–	–
Catalog	2	200	–	–	–	–
Photo Copy	3	4	77	–	–	–
Journals	4	80	125	64	–	–
New Books	5	32	42	19	26	–

The numbers in the matrix represent the number of trips from facility i to facility j. We would like to locate the departments so as to maximize the sum of the values of *adjacent* pairs of departments. Each department is a vertex of a complete graph, with the number of trips being the weight on each arc. The solution is to find the planar sub-graph that contains all the vertices and has the maximum total weight. Figure 6.20 shows both the graph and the max spanning tree for this problem.

Traveling Salesman Problem

Please, do not read the text book for this problem. Consider the following distance matrix.

$$\left[\begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & a & c & M \\ 2 & & 0 & b & e \\ 3 & & & 0 & a \\ 4 & & & & 0 \end{array}\right]$$

The matrix need not be symmetric, c_{ij} need not equal c_{ji}. The distance matrix contains more information than the node incidence matrix because it tells you the nodes are connected and by what amount. M

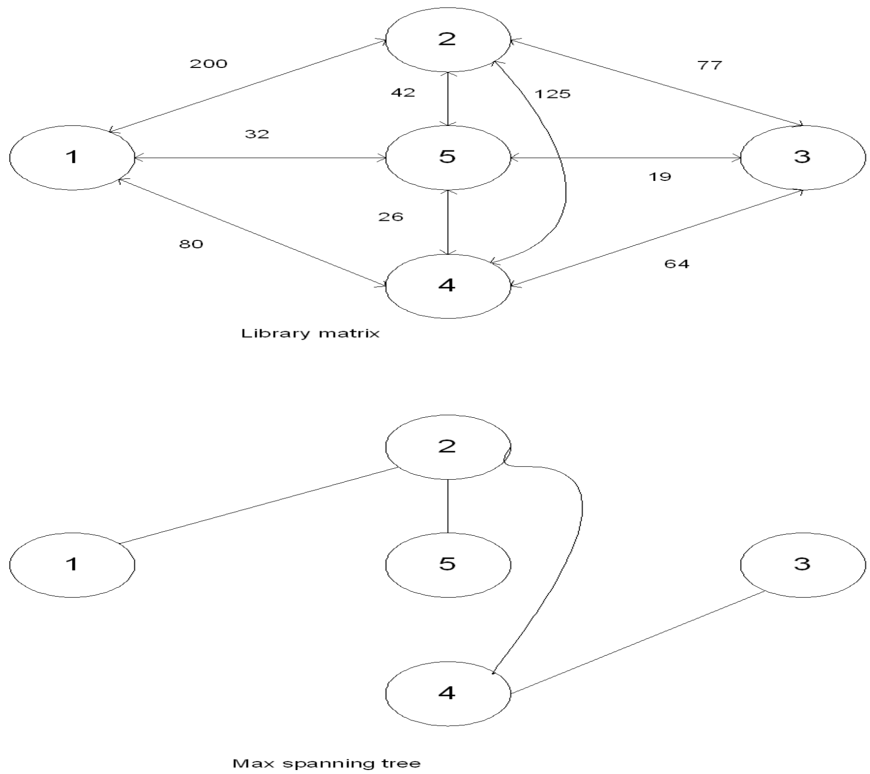

Figure 6.20: The library example.

means no connection, but does not translate into a matrix directly. The distance matrix is all we need for the traveling salesman problem. We want to find the single path from the starting node 1 back to it which passes through every other node exactly once and minimizes the total distance. This sounds easy, but is not an easy problem to solve.

6.4 Constructing Project Network Diagrams

This section lists the rules for constructing project network diagrams.

1. Each activity is represented by one and only one arrow in the network.

2. No two activities may be represented by the same head and tail node. Must introduce a dummy activity.

In project networks, CPM is used more often tan PERT because it is more simplistic and PERT has some unrealistic assumptions.

Example: Building a house.

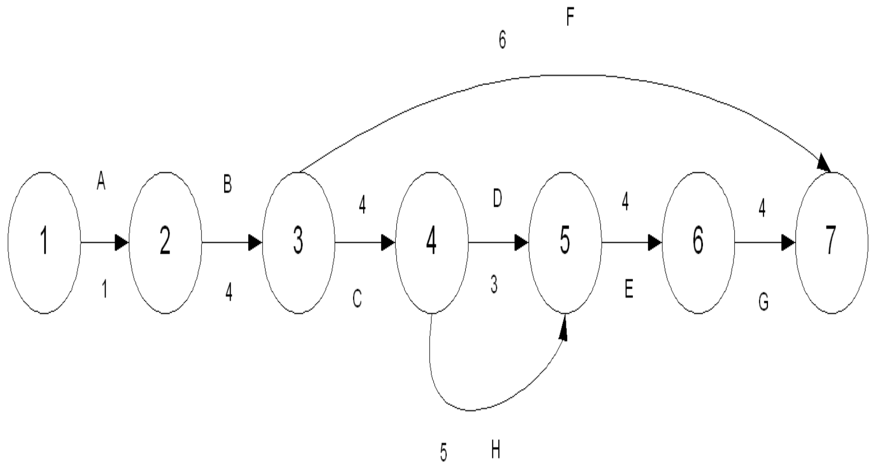

Figure 6.21: The building a house example.

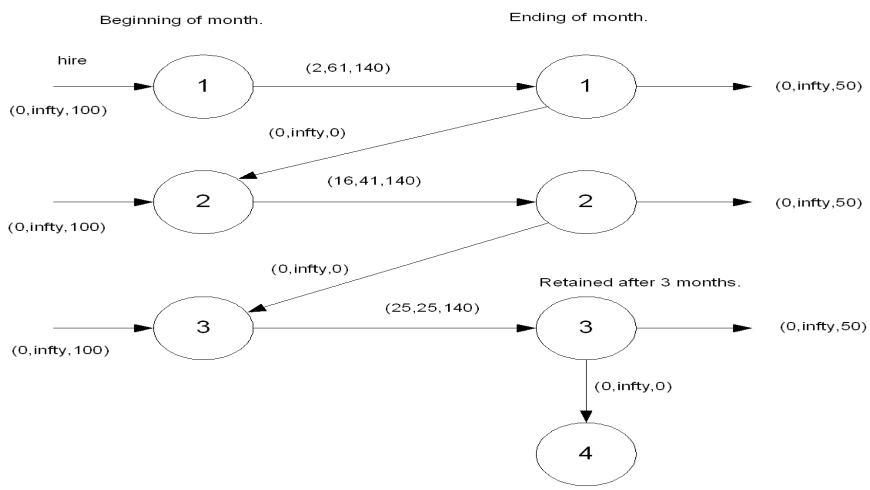

Figure 6.22: The hiring and firing example.

	Activity	Predecessor	Time
A	Clean Land	$\emptyset$	1
B	Lay Foundation	Clean Land	4
C	Frame Walls	Lay Foundation	4
D	Wire	Frame Walls	3
E	Install Drywall	Lay Foundation	4
F	Landscape	Lay Foundation	6
G	Interior Work	Install Drywall	4
H	Roof	Frame Walls	5

The critical path is the one which if it is delayed, then the entire project is delayed. We will be looking for the longest path. Consider the network in Figure 6.21. Note that the parallel arcs D and H can be combined into one arc. Or, if you want to keep them separate, replace one of the arcs by two arcs in sequence. This type of network is called *activity on the arc (AOA).*

Problem: How do you represent float? $x_{12} + x_{13} + x_{14} = 20$ on the network? You can't seem to do that. Consider the network in Figure 6.22. Now, with this problem we cannot show the cost of going from node 1 to 4. How does this problem differ from the usual transshipment problem? We don't have an exact requirement, we have a maximum and a minimum.

Example: An employee hiring and firing problem. It costs \$100 per worker to hire; \$50 per worker to fire; and \$140 per worker per month in salary. Presently, there are zero workers on hand.

Month 1	20
Month 2	16
Month 3	25

Determine a hiring and firing strategy. Stated as an LP problem, $\min(z) = 50(x_{12} + x_{13} + x_{23}) + 100(x_{12} + x_{13} + x_{14} + x_{23} + x_{24} + x_{34}) + 140(x_{12} + x_{23} + x_{34}) + 280(x_{13} + x_{24}) + 420x_{14}$. x_{ij} is the $i - th$ hire at the end of month $j - 1$. So, x_{14} represents months 1, 2, 3. The $\min(z)$ is subject to 1) $x_{12} + x_{13} + x_{14} \geq 20$, 2) $x_{13} + x_{14} + x_{23} + x_{24} \geq 16$, and 3) $x_{14} + x_{24} + x_{34} \geq 25$. $x_{ij} \geq 0$. You need to manipulate this problem to get the network formulation.

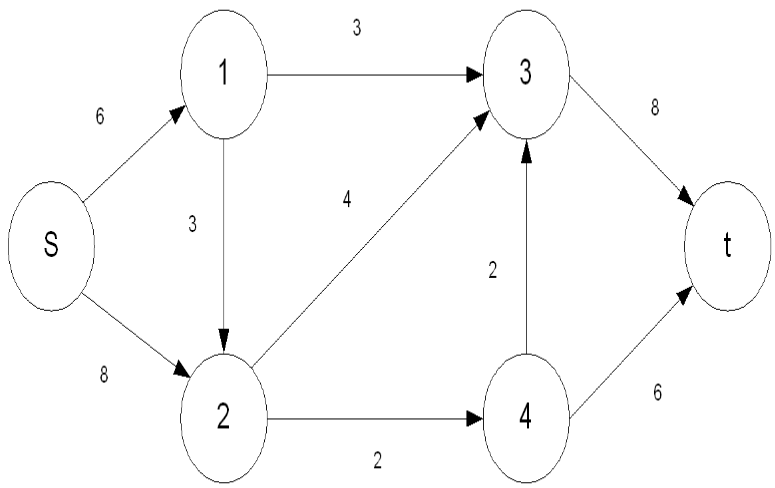

Figure 6.23: A maximum flow example.

This section deals with sending the maximum flow through a network. One unit at a time may not always be the best way. The capacity constraints are the upper and lower bounds. See Figure 6.23 for an example. Assume the numbers are costs. How can we formulate this as an LP problem?

$$x_{S1} + x_{S2} - V = 0,$$

$$x_{13} + x_{12} - x_{S1} = 0,$$

$$x_{23} + x_{24} - x_{32} - x_{12} = 0,$$

$$x_{3t} - x_{43} - x_{23} - x_{13} = 0,$$

$$x_{43} + x_{4t} - x_{24} = 0,$$

$$V - x_{3t} - x_{4t} = 0.$$

We want to maximize V which is the interim flow in and out of the nodes. The arc capacity constraints are $x_{s1} \leq 6$, $x_{s2} \leq 8$, $x_{12} \leq 3$, $x_{23} \leq 4$, $x_{24} \leq 2$, $x_{3t} \leq 8$, $x_{4t} \leq 6$.

The general LP formulation is given by $\max(V)$ subject to

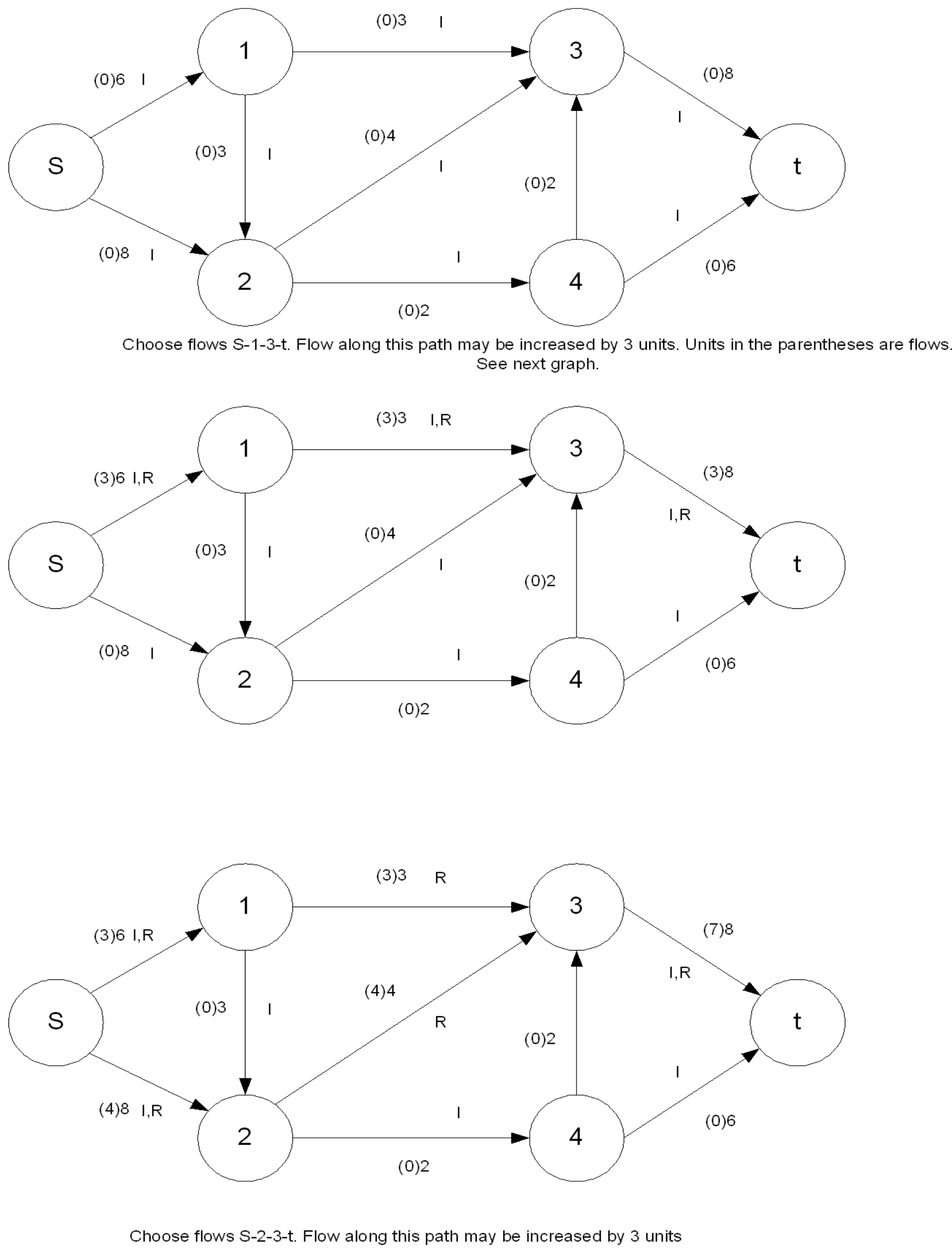

Figure 6.24: An algorithm trace for finding the max flow.

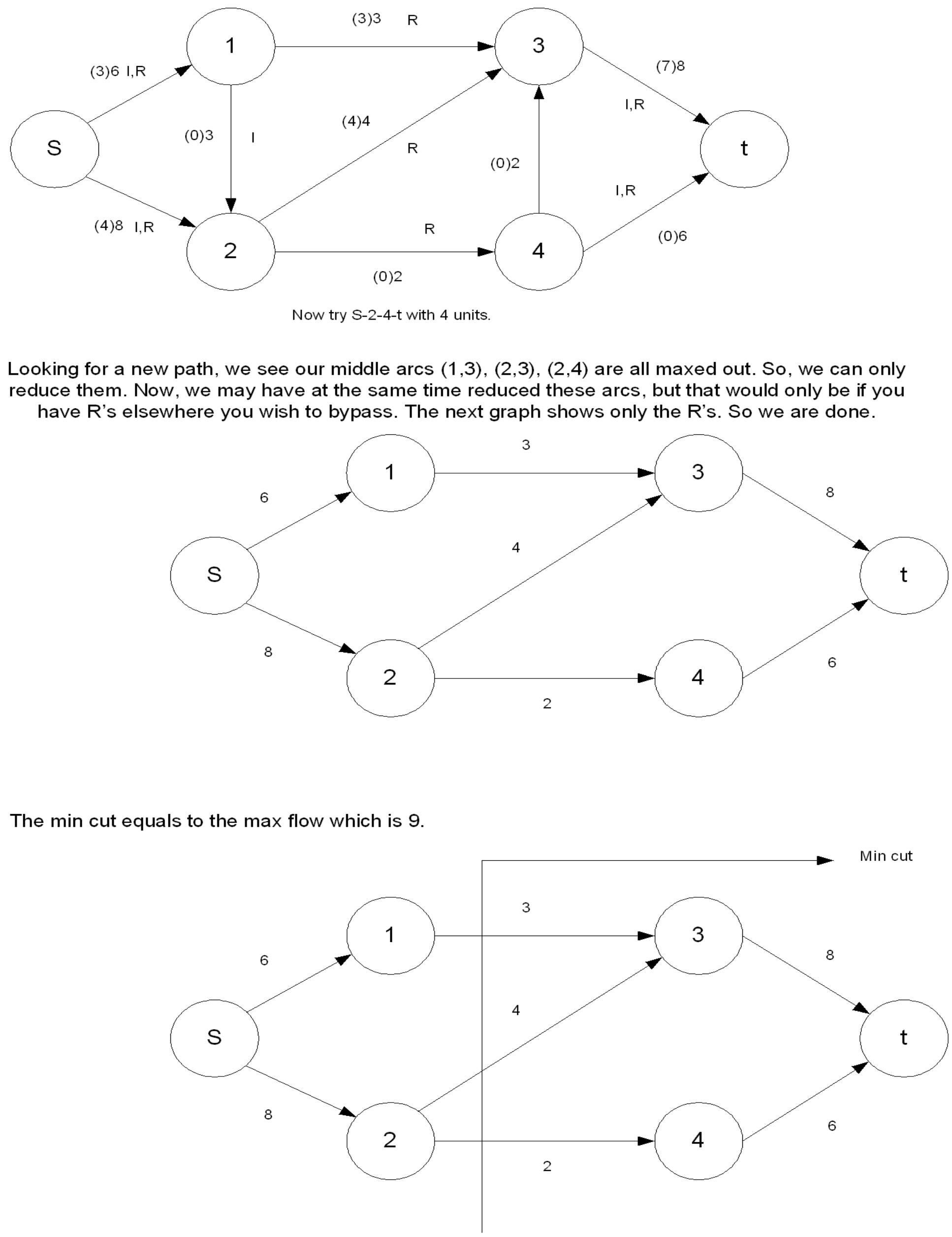

Figure 6.25: The final algorithm trace for finding the max flow.

$$\sum x_{ij} - \sum x_{ji} = 0, \forall i \neq s, t$$
$$\sum x_{sj} - \sum x_{js} = V$$
$$\sum x_{jt} - \sum x_{tj} = V$$
$$0 \leq x_{ij} \leq U_{ij}.$$

A better way to solve the max flow problem is to use the Ford-Fulkerson (1962) method. The underlying idea is to start with any flow from S to t. Look for a flow augmenting path. If you find one, send as many units as possible, then look for another. Stop when no more such paths exist. Let's use Figure 6.23 for an example. Let I represent the set of arcs with additional capacity. Let R be the set of arcs whose current flow can be reduced. Can an arc be in both sets? Yes, if they are undirected arcs or if they are directed arcs where you allow for reverses for the purpose of making an answer more feasible. See Figure 6.24 and Figure 6.25 for determining the sets I and R. You can use the max flow algorithm and min cut algorithm to verify the results.

Maximum Flow Extensions

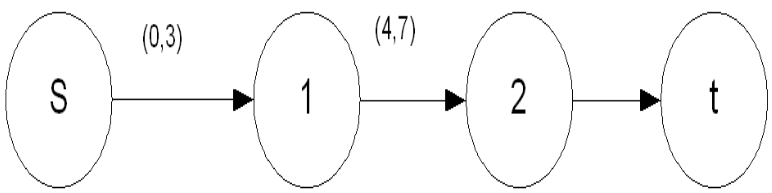

Figure 6.26: An example where a lower feasible bound may not exist.

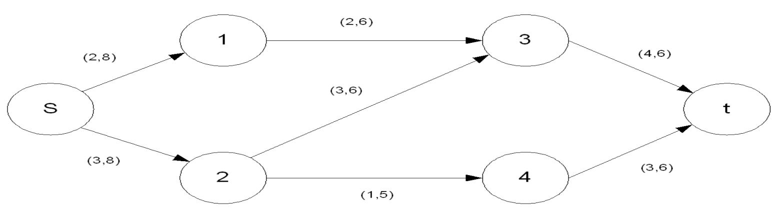

Figure 6.27: An example of transforming a given network so that all the lower bounds are zero.

Suppose we have several sources and sinks. Then, we must make a super source and a super sink with those arcs. The upper bounds are the capacities, and the lower bounds are the demand amounts. In some cases a feasible lower bound may not exist. Consider Figure 6.26. If we have a feasible flow, how can we find the max flow? Note: Before we looked only at the minimum of the max. Now we are looking at the maximum of the min too. Can we transform the network in Figure 6.27 into an equivalent one with the lower bounds of zero, then apply our algorithm? Yes, see Figure 6.28. Another idea is to subtract the lower bound out of both bounds, and solve with the max flow algorithm. See Figure 6.29.

See Figure 6.30 for the oil refinery example. This example is on page 255 of the text book. There are three oil refineries, and two sources: Alaska at \$0.40/gal and Persian Gulf at \$0.30/gal. Both sources can furnish a minimum of 300,000 gals/day with no maximum. Must use both sources. The following tables contain the data.

The distribution costs and production are in the following table.

Refinery	Ref. Cost	Max Prod.	Min Prod.
1	0.03	1250,000	200,000
2	0.04	1500,000	300,000
3	0.05	1350,000	300,000

The shipping costs are in the following table.

Ref.	NY	Alt.	Dal.	LA
1	0.05	0.06	0.06	0.02
2	0.06	0.07	0.07	0.06
3	0.07	0.06	0.06	0.05

The daily requirements are in the following table.

Location	Max Demand	Min Demand	Sell Price
NY	250,000	200,000	0.85
Alt	175,000	90,000	0.70
Dal	175,000	100,000	0.65
LA	350,000	200,000	0.75

The arcs represent (max, min, $ per unit). We get the arc (4,1) because this is required to use the out of kilter algorithm. You need to have a closed network. See the text book for the rest of the numbers. The sales number is a regular number on the network because the dollars numbers on the network represent costs. The solution is $-29,525.00$ meaning the profit is $29,525. Arc(1,2) + Arc(1,3) $= 950, \ldots$ Arc(10,14) + Arc (11,14) + Arc(12,14) + Arc(13,14) $= 250 + 175 + 175 + 350 = 950$.

Example: An MCNFP example to determine the service districts. A region has two hospitals which serve as bases for emergency medical vehicles. Two ambulances are at hospital 1 and three are at hospital 2. The hospitals operate independently. The region has been partitioned into 10 areas, each independently generating calls at a rate of r_i per hour for area i. The average service time (not travel time when you are on site) for a call is 0.50 hours and the total rate at which calls arrive is 3 per hour (assume it is exponential).

		Ave. Time	
Area	Call Rate	Hosp 1	Hosp 2
A_1	0.2	2.0	6.0
A_2	0.3	2.0	5.5
$\vdots$	$\vdots$	$\vdots$	$\vdots$
A_{10}	0.3	6.5	4.0
	3.0 calls/hr		

How should areas be assigned to hospitals so that the average response time is minimized while insuring that the probability that a call incurs a queuing delay less than 10%? See Figure 6.31. Note, we have two independent queues, one with a size of 2, and the other with a size of 3. Given, $W = 0.5$ hours, solve for the λ which makes p_2 and p_3 respectively equal to 0.1 (10%). You get $\lambda = 1.0$ for $s = 2$ and $\lambda = 2.1$ for $s = 3$. The delay problem depends on the total call rate assigned to each hospital. Using a simple queuing model with a service time of 0.5 hours, the maximum call rate yielding a delay probability of 10% is approximately 1.0 for two servers and 2.1 for three servers. Suppose this sum had been 1.6 instead of 3.1. Can't meet the rate of 10% with the total calls being 3.0 per hour. So you need to make some changes. Suppose that the 10% had not been given? Then solve the queue for a total rate of 3.0.

Back to the PERT/CPM models. To ensure the correct precedence relationships, answer the following questions as every activity is added to the network.

1. What activities must be completed immediately before this activity can start?
2. What activities must follow this activity?
3. What activities must occur concurrently with this activity?

Event numbering rules:

1. Give the start event the number 1.
2. Give the next number to any un-numbered event whose predecessor events are not already numbered.
3. Repeat Step (2) until all nodes are numbered. The finish node will always receive the highest number.

See Figure 6.32.

Example: Consider the following table.

Activity	Predecessors
A	$\emptyset$
B	A
C	A
D	A
E	B, C
F	B, C, D
G	E, F

See Figure 6.33 for the proper labeling of the activities.

Example: Job A precedes jobs B and C. Jobs C and D preceed job E. Job B precedes job D. Jobs E and F preceed job G.

Activity	Predecessors
A	$\emptyset$
B	A
C	A
D	B
E	C, D
F	$\emptyset$
G	E, F

See Figure 6.34 for the incorrect and correct labeling of the arcs and nodes.

Example: Consider the following table.

Job	Predecessors	Times
A	$\emptyset$	3
B	$\emptyset$	1
C	A	4
D	A, B	2
E	C, D	5

See Figure 6.35 for the correct labeling of the arcs and nodes.
The critical path is the longest path through the network because those events on the critical path are the events that affect the total project time.

6.4.1 LP Formulation

Let x_{ij} be the time for the event corresponding to node j occurs. Thus, for each activity (i, j), $x_j \geq x_i + t_{ij}$. The objective function is $z = x_F - x_1$. We wish to minimize the objective function which is the same as minimizing the finish time and start time subject to $x_j \geq x_i + t_{ij}, \forall(i, j)$. Sometimes it will be free because of the dual is the longest path in the network.

Example: This example is the same as the previous example. Let t_i represent the time at which event (node) i occurs where $i = 1, 2, .., 5$. For example, t_5 is the completion time whereas t_4 represents the time at which both jobs C and D are completed. Thus, $t_5 - t_1$. Minimize the time of completing the project. $\min(z) = t_5 - t_1$, subject to $t_2 - t_1 \geq 3$, $t_3 - t_1 \geq 1$, $t_3 - t_2 \geq 0$, $t_4 - t_2 \geq 4$, $t_4 - t_3 \geq 2, t_5 - t_4 \geq 5$.

Note: You could let $t_1 = 0$ and delete it from these equations. This is in fact what LINDO does. Solution: $t_1 = 0, t_2 = 3, t_3 = 3, t_4 = 7, t_5 = 12$ So, $z^* = 12$ days. How is the critical path calculated? It is composed of those activities whose constraints are satisfied by the equalities of the solution. Recall the constraints, $t_2 - t_1 \geq 3, 3 - 0 = 3(c^*), t_3 - t_1 \geq 1, 3 - 0 \geq 1, t_3 - t_2 \geq 0, 3 - 3 = 0(c^*), t_4 - t_2 \geq 4, 7 - 3 = 4(c^*), t_4 - t_3 \geq 2, 7 - 3 \geq 2, t_5 - t_4, 12 - 7 \geq 5 = 5(c^*)$. Therefore, the critical path is $t_1 \rightarrow t_2 \rightarrow t_4 \rightarrow t_5$. What is the slack? It is what is left over from the greater-than or equal signs. So the slack is $2 + 2 = 4$.

Example: Curriculum programming as a project network. To get a degree in OR, the following courses are required.

1. Calculus I, and II.
2. Statistics I, and II.
3. Linear Programming.

   Non-Linear Programming.
4. Stochastic Programming.

The precedent requirements are

1. Calculus I before Calculus II.
2. Statistics II and Calculus II before Statistics III.
3. Calculus I before Statistics I.
4. Statistics I before Statistics II.
5. Calculus II and LP before Non-Linear Programming.
6. Calculus II, Statistics II, and LP before Stochastic Programming.

See Figure 6.36. The critical path is the number of semesters.

Semester	Course
1	LP, Calculus I
2	Statistics I, Calculus II
3	Statistics II, Non-LP
4	Statistics III
5	Stochastic Programming

6.5 CPM Models

For the numbering of nodes, an earlier activity should have a smaller node number than an later activity. Figure 6.37 shows one possible node numbering scheme. Figure 6.38 shows a better node numbering scheme. In this problem, there are only three paths through the network. See Figure 6.39.

Path	Length
$A-B-F$	11
$A-B-C-D-E-G$	20
$A-B-C-H-E-G$	22$*$

The last path with a length of 22 is the critical path since it is the longest. For solving this problem, in general, do not enumerate all possibilities. Solve using a modified Dijkstra's algorithm for finding the longest route. ET is the earliest time an event can occur. $ET(i)$ is the earliest time one could "leave" node i. $LT(j)$ is the latest time one could leave node j without delaying the completion time. If an arc/activity i is on the critical path, then $ET(i) = LT(j)$.

Consider Figure 6.40. In the forward pass, compute the earliest occurrence. In the backwards pass, compute the latest occurrence. From node 2, with nodes 0, 1, and 2 being labeled, we must go to node 3 next. We cannot go to node 4 because there is an arc going into node 4 (from node 3) that is from an unlabeled node as of yet. The earliest occurrence for node 3 is the *earliest time* when all activities going into node 3 are completed. So, we are choosing the *largest* choice. In the forward pass, we must make sure the arcs leaving node "A" to nodes to the other nodes have labels before labeling node "A." Choose the smaller of the two going backwards. How do we get the critical path? The critical path consists of the arcs (i, j) such that the following three conditions are satisfied.

1. $ET(i) = LT(i)$.
2. $ET(j) = LP(j)$.
3. $ET(j) - ET(i) = LT(j) - LT(i) = t_{ij}$ where t_{ij} is the activity time on arc (i, j).

Floats: In this case, the total float is equal to the free float for all activities except $(0, 1)$. The total float $TF(i, j)$ is the amount of time that starting time of (i, j) could be delayed with delaying the completion of the project. $TF(i, j) = LT(j) - ET(i) - t_{ij}$. Any activity with a total float of 0 is a critical activity. Any path from the start to the finish consisting exclusively of critical activities is called the *critical path.* The *free float* $FF(i, j)$ is the amount by which starting at time of (i, j) or duration of its activity, can be delayed without delaying the start of any later activity beyond its earliest possible starting time. So, $FF(i, j) \leq TF(i,)$. Also, $FF(i, j) = ET(j) - ET(i) - b_{ij}$. The total float is more important to us.

Getting back to the example, $TF = FF$ except with (0, 1). So, 'F' means total floats. $F(0, 1) = 2$, $FF(0, 1) = 0$, $F(1, 3) = 2$, F(2,4) = 1, $F(4, 6) = 8$, $F(3, 5) = 4$, $F(3, 6) = 11$.

6.5.1 Time Charts

We can create a time chart showing activities according the following rules.

1. The critical activities are solid lines. The non-critical activities are dashed lines.
2. If $FF(i, j) < TF(i, j)$, then (i, j) can be delayed past $ET(i, j)$ no more than $FF(i, j)$ without affecting the next activities.

3. If $TF(i,j) = FF(i,j)$ then the non-critical activity can be scheduled anytime. So we have $ET(i,j)$ and $LT(i,j)$.

In our example, (0,1) must start at time 0. Otherwise, (1,3) is delayed. See Figure 6.41.

Is the critical path fixed? This is not always the case. There are certain ways of speeding up an activity at a cost. "Crashing" may sometimes be possible. Crashing refers to the shortening of an activity's duration by spending money. Sending manuals by special order, using OT hours, hire more people, etc. The additional cost is referred to as the "crashing cost." Why would you consider crashing? You might be able to save other costs. Like, avoid late penalties, shorten equipment rental time, increase sales b/c first on the market, or reduce supervisor costs. The critical path method allows us to make trade offs between the total cost of a project and it completion time.

Example: An example of a project network with crashing allowed. Let's compare two methods: 1) Enumeration, and 2) LP.

Job	Predecessor	Nornal Time	Crash Time	Cost to Crash per Day
A	–	10	7	4
B	–	5	4	2
C	B	3	2	2
D	A, C	4	3	3
E	A, C	5	3	3
F	D	6	3	5
G	E	5	2	1
H	F, G	5	4	4

The overhead costs are \$5.00 per day. What is the optimal duration of the project in terms of both crashing and overhead costs? Develop an optimal project schedule. See Figure 6.42.
The arcs represent $[ET(i), LT(j)]$. There are two alternative paths that are critical. If all jobs were "crashed" to the maximum, then the project duration would be 17 days. The optimal time will be $17 \leq T \leq 25$. The cost with no crashing is $\$125.00 = 5 \times 25 + 0$. The cost with crashing is $\$132 = 5 \times 17 + 47$. Can we do better than \$125.00? Using normal times for the jobs, the earliest and latest occurrence times of the events were completed. There were two critical paths. See Figure 6.43 and Figure **??**.

The critical activities are jobs A, E, E, F, G, H. The cost with no crashing is \$125.00. To reduce the duration of the critical jobs, consider the critical job H which can be crashed by 1 day at a cost of \$4.00. This reduces the total project time by 1 day at a savings of \$5.00 in overhead costs. Hence job H is crashed to its lower limit (4 days) and the total cost is reduced to \$124.00. Now consider job A. If it were crashed, there is a net savings of \$1.00 for each day crashed. But job A cannot be crashed to its minimum value of 7 days because when A is crashed to 8 days, then jobs B and C also become critical. See Figure 6.44.

So, it would not help for arc A's duration to be reduced to 7. Thus, job A should be crashed only to 8 days and the total cost is reduced to \$122.00. So now, we have a parallel critical path (A, and B&C). If we reduced the arc A's duration by 1 day, we would have to reduce B or C by 1 day as well. The total cost of crashing here is \$6.00 which exceeds \$5.00 of overhead per day. Therefore it is not worth crashing. Now consider jobs D, E, F, and G. See Figure 6.45. Since we have a parallel critical path between nodes 3 and 6, we have to crash one of the jobs in the path. So, as you can see, D for path 1 and G for path 2 are the most beneficial crashes. And, $D + G = 4 < \$5.00$ in overhead costs. So, crash D and G by 1. Now, G cannot be crashed any lower — it's at it's crash limit. The only other crash possibilities for the two critical paths would be $3 + 3 = 6 > 5$ or $3 + 5 = 8 > 5$. So, we are done. The cost of \$121.00 is the optimal solution: crash job A to 8 days; crash job D to 3 days; crash job G to 4 days; crash job H to 4 days. The optimal length is 21 days.

This technique is inefficient but under the assumption that each day's crashing cost is the same for each activity i (i.e. the cost is linear), then the problem can be solved as an LP. Also assume we can work partial days! If the problem does not allow partial days, the solve as an LP problem. If the costs are non-linear, the do not use the LP.

6.5.2 LP Formations for Optimal Crashing

The notation that we will use is as follow: k_{ij} is the normal completion time of (i, j). l_{ij} is the crash completion time with a maximum amount of resources of (i, j). c_{ij} is the unit cost of shortening the duration of jobs (i, j) by 1 unit of time. t_{ij} is the completion time of job (i, j) where $l_{ij} \leq t_{ij} \leq k_{ij}$. The cost of crashing is $c_{ij}(k_{ij} - t_{ij})$. Let t_i be the unknown event times $(i = 1, 2, ..., n)$ for a project consisting of n events, where 1 and n are the start and end nodes, respectively. The three LP models can be developed.

1. The minimum crash cost is subject to being less than or equal to the finish time T.

   $$\min z = \sum_{(i,j)} c_{ij}(k_{ij} - t_{ij})$$

   subject to

   $$t_j - t_i \geq t_{ij}, \forall \text{ jobs } (i, j),$$
   $$l_{ij} \leq t_{ij} \leq k_{ij}, \forall \text{ jobs } (i, j),$$
   $$t_n - t_i \leq T,$$
   $$t_{ij}, t_i \geq 0, \forall i = 1, 2, ..., n$$

   Note: To be feasible, T must be greater than or equal to the project duration when all activities are crashed.

2. The minimum completion time is subject to the crash cost being less than or equal to B, the budget. The minimum project duration subject to the crash budget of \$B.

   $$\min z = t_n - t_1,$$

   subject to

   $$\sum c_{ij}(k_{ij} - t_{ij}) \leq B$$
   $$b_j - t_i \geq t_{ij}, \forall \text{ jobs } (i, j),$$
   $$l_{ij} \leq k_{ij}, \forall \text{ jobs } (i, j),$$
   $$t_i, t_{ij} \geq 0, \forall i, j.$$

   By solving models I and II repeatedly, we could obtain the relationship for the project cost and the project duration. T^* can be found using model III which minimizes the total cost. Using the notation of models II and I, formulate model III. We need to include the over head cost in model III (we've included this implicitly in I and II by the upper bound k_{ij}; but now wee must show it explicitly).

3. The minimum is total overhead cost plus the crash cost. Minimize the over head cost and the direct crashing cost. Let F (for fixed) be the over head cost per day. It does not vary from day to day. Then, the over head cost is $F(t_n - t_1)$.

   $$\min F(t_n - t_1) + \sum_{(i,j)} c_{ij}(k_{ij} - t_{ij}),$$

subject to

$$t_j - t_i \geq t_{ij}, \forall \text{ jobs } (i,j),$$

$$l_{ij} \leq t_{ij} \leq k_{ij}, \forall \text{ jobs } (i,j),$$

$$t_{ij}, t_i \geq 0, \forall i = 1, 2, ..., n.$$

Recall the previous example (without crashing). The LP is formulated as $\min 5(t_7 - t_1) + 4(10 - t_{13}) + 2(5 - t_{12}) + 2(3 - t_{23}) + 3(4 - t_{34}) + 3(5 - t_{35}) + 5(6 - t_{46}) + 1(5 - t_{56}) + 4(5 - t_{67})$, subject to

$$\begin{array}{ll}
t_3 - t_1 \geq t_{13} & 7 \leq t_{13} \leq 10 \\
t_2 - t_1 \geq t_{12} & 4 \leq t_{12} \leq 5 \\
t_3 - t_2 \geq t_{23} & 2 \leq t_{23} \leq 3 \\
t_4 - t_3 \geq t_{34} & 3 \leq t_{34} \leq 4 \\
t_5 - t_3 \geq t_{35} & 3 \leq t_{35} \leq 5 \\
t_6 - t_4 \geq t_{46} & 3 \leq t_{46} \leq 6 \\
t_6 - t_5 \geq t_{56} & 2 \leq t_{56} \leq 5 \\
t_7 - t_6 \geq t_{67} & 4 \leq t_{67} \leq 5
\end{array}$$

The optimal solution is $t_1 = 0, t_2 = 5, t_3 = 8, t_4 = 11,\ t_5 = 13, t_6 = 17, t_7 = 21, t_{13} = 8,\ t_{12} = 5, t_{23} = 3,$ $t_{34} = 3, t_{35} = 5, t_{46} = 6, t_{50} = 4, t_{67} = 4$. So, $F^* = \$121.00$ where all the nodes are critical activities with the optimal solution. Activity A is crashed 2 days, and activities D, G, H are crashed 1 day.

6.6 Activity on the Node Networks

For the examples, see page 287 of the text book. Most text books do not cover Activity on the Node Network, but our's does.

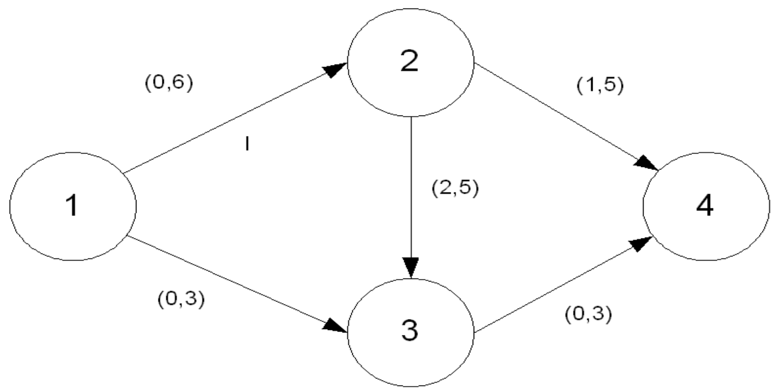

Figure 6.28: An example of transforming a given network so that all the lower bounds are zero.

Figure 6.29: An example of subtracting the lower bound from both the upper and lower bounds.

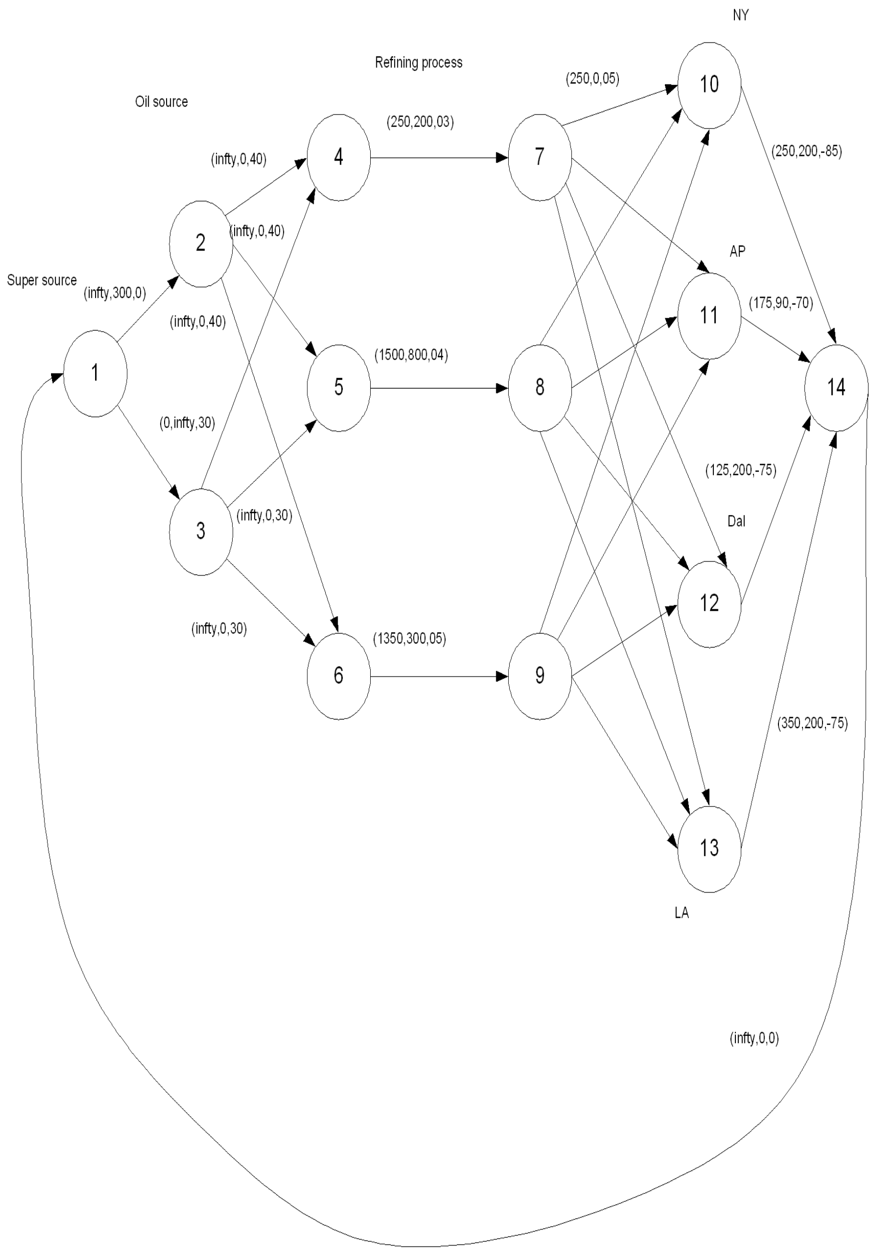

Figure 6.30: The oil refinery example in the text book.

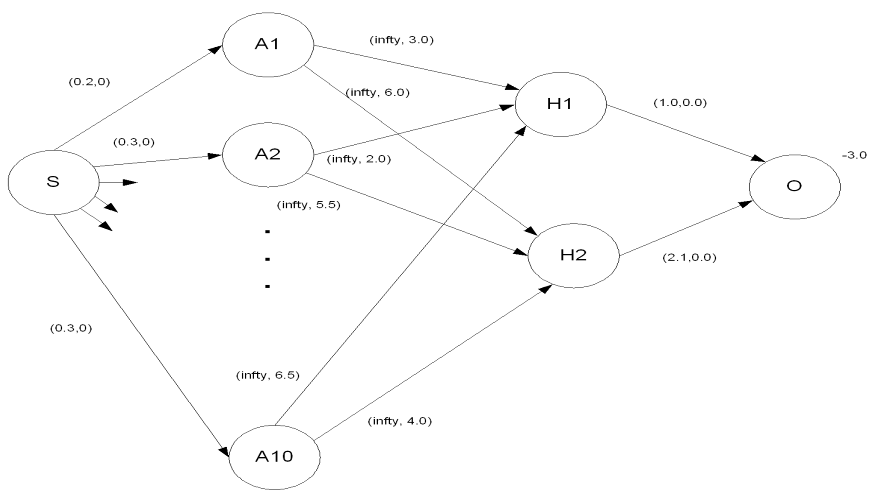

Figure 6.31: The hospital example.

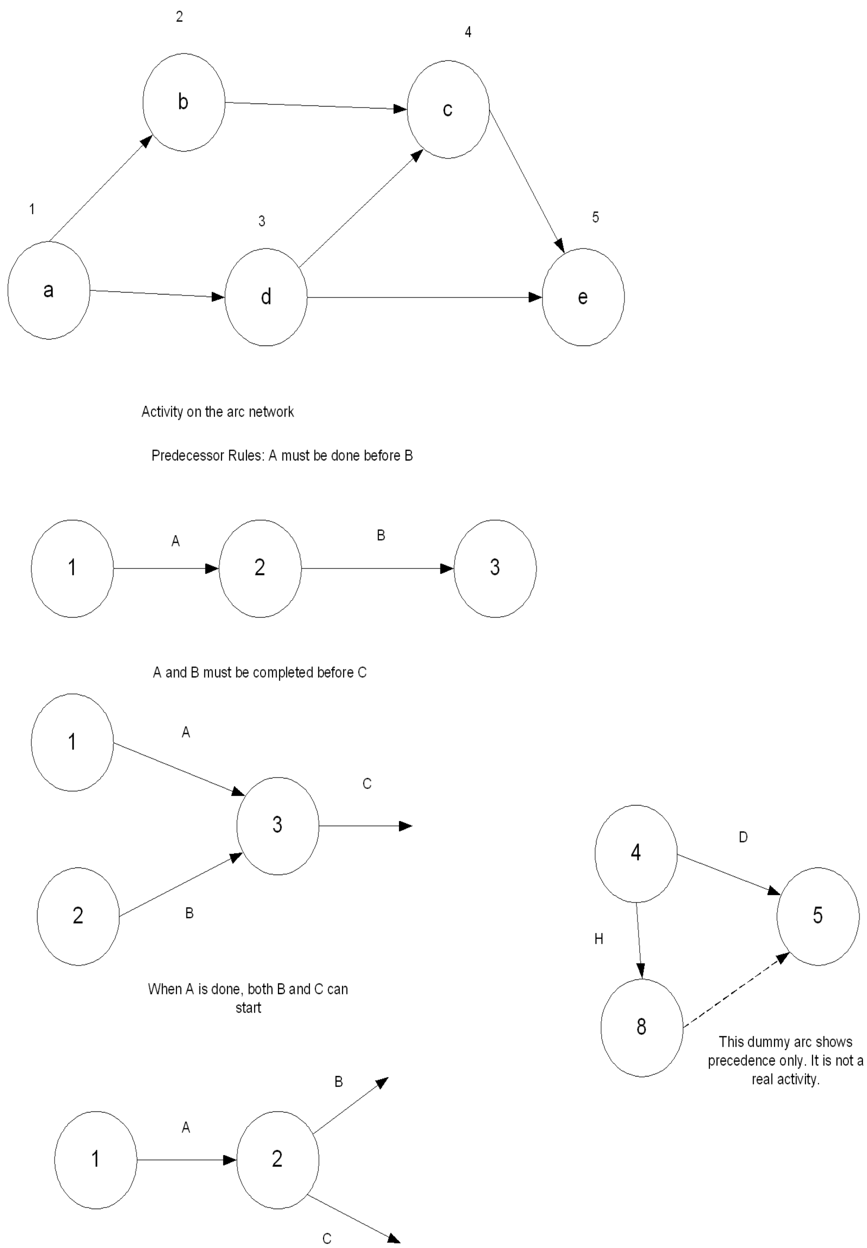

Figure 6.32: Shows the rules for labeling relationships for activities on the arc networks.

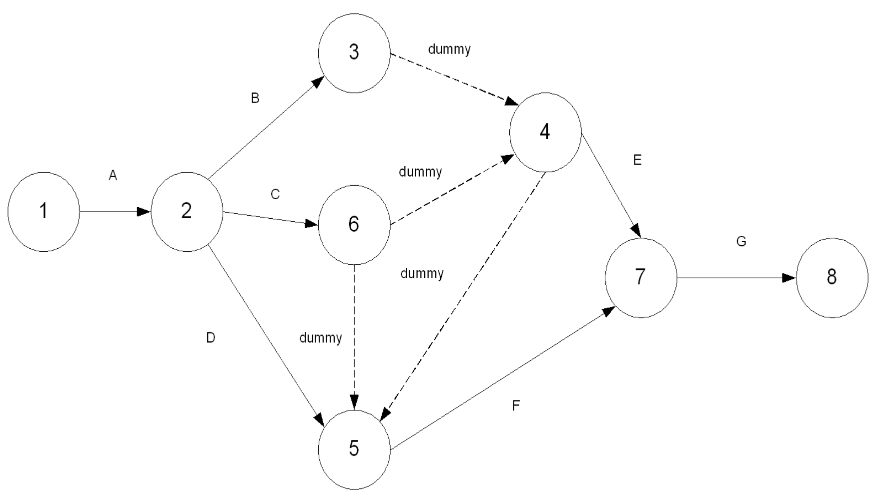

Figure 6.33: A network example with dummy activities on the arcs.

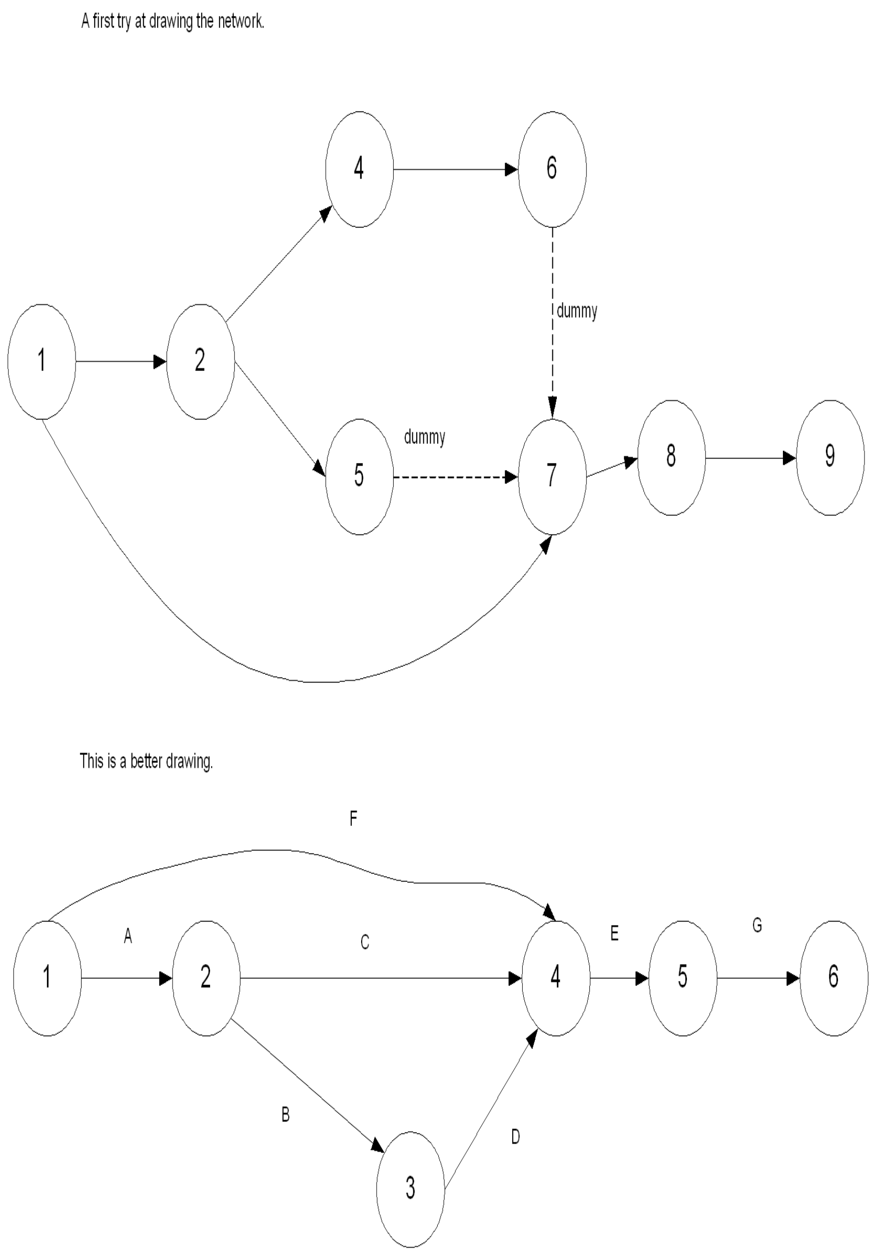

Figure 6.34: Two examples of drawing the same network. The network on the bottom is the better of the two.

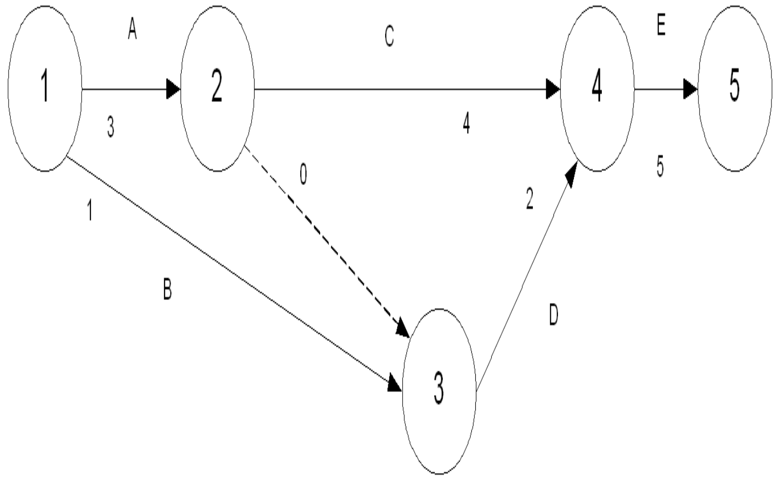

Figure 6.35: Another example of labeling arcs and nodes.

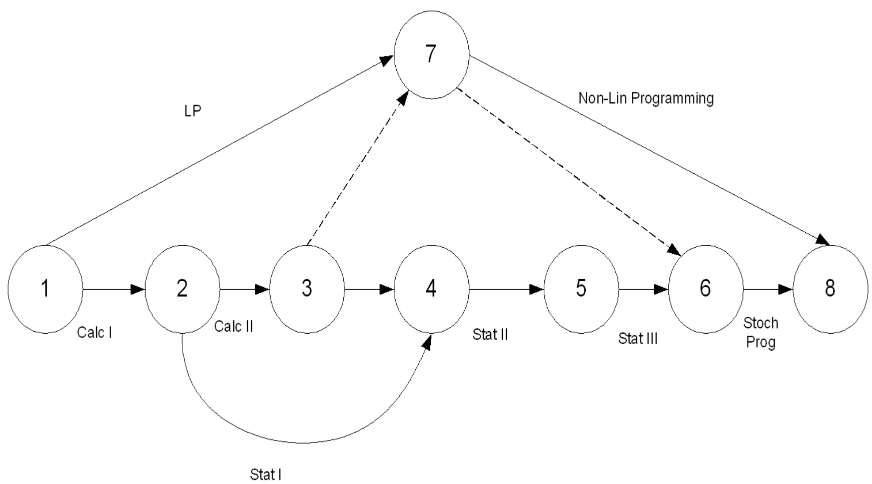

Figure 6.36: A network showing the courses and semesters.

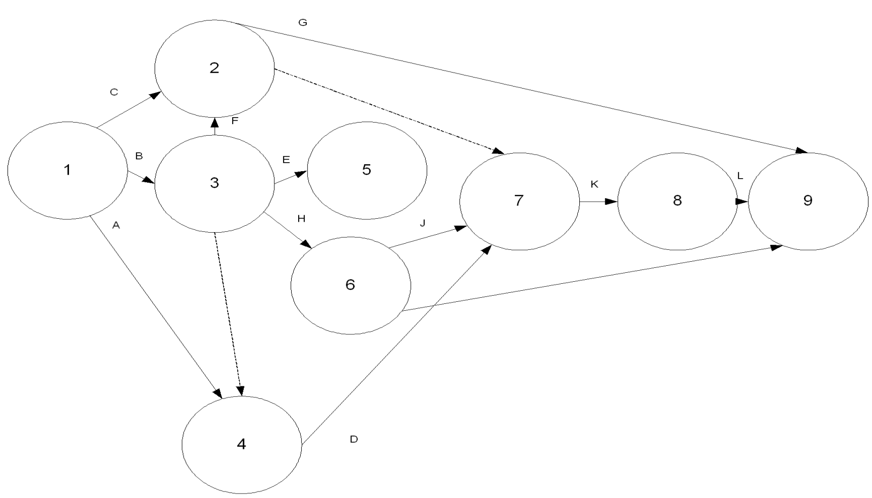

Figure 6.37: Less than desirable node numbering.

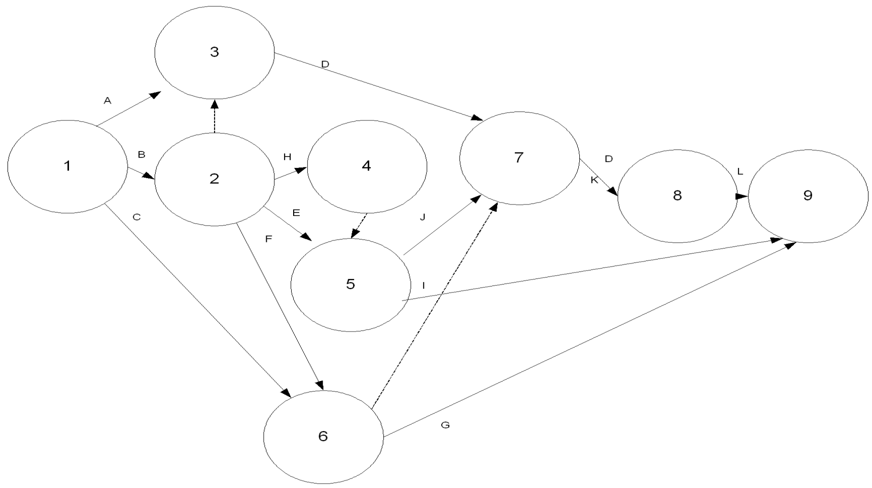

Figure 6.38: A better node numbering scheme.

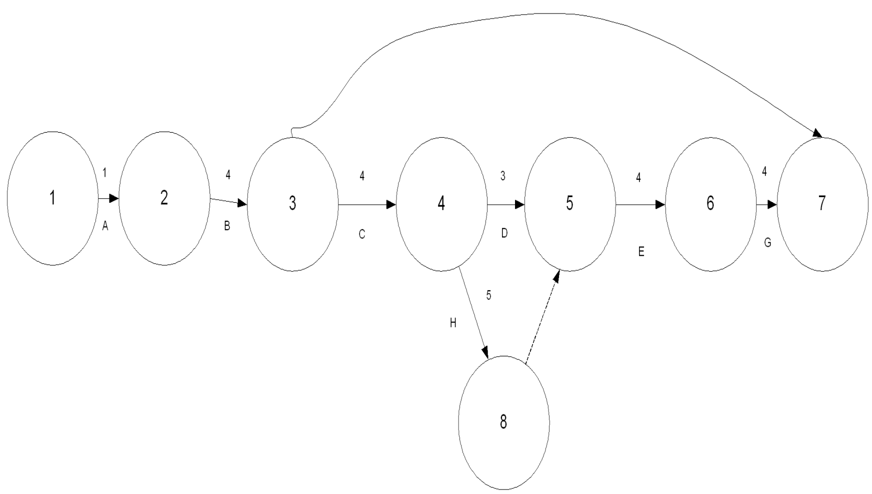

Figure 6.39: Example of a Critical Path Problem

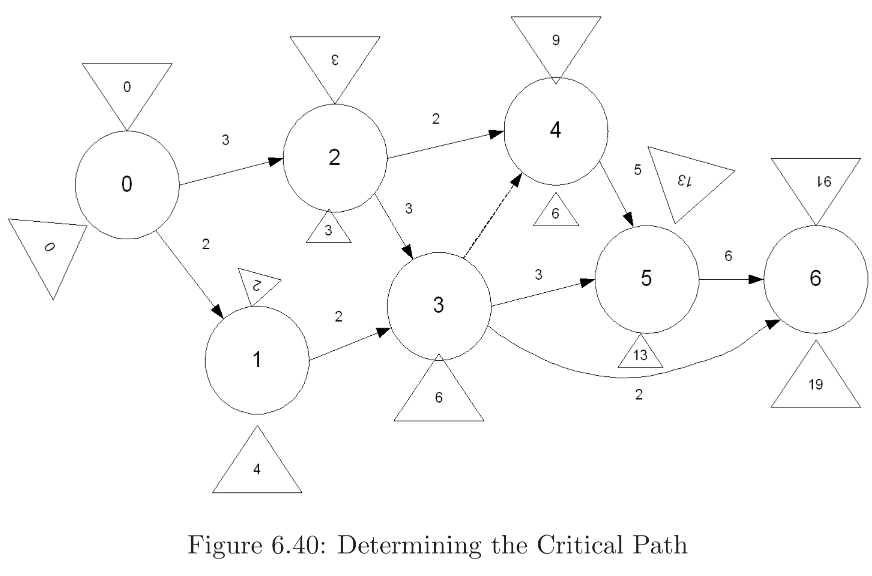

Figure 6.40: Determining the Critical Path

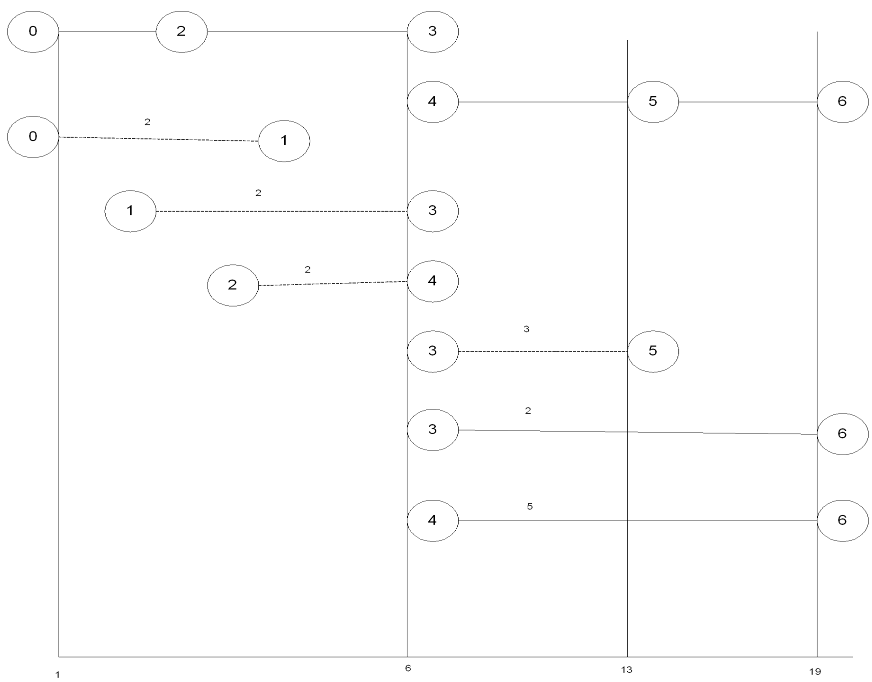

Figure 6.41: A Time Chart.

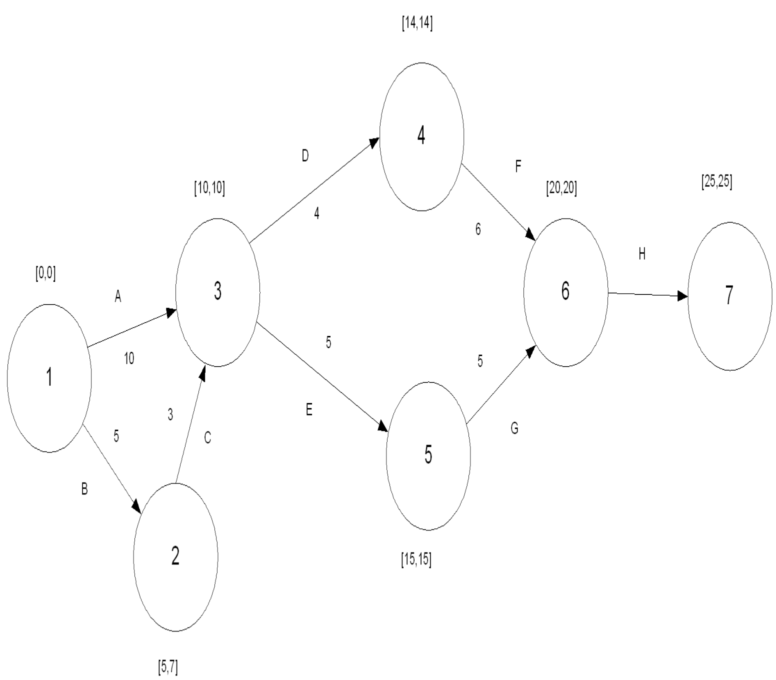

Figure 6.42: Trade offs between crash costs and overhead costs.

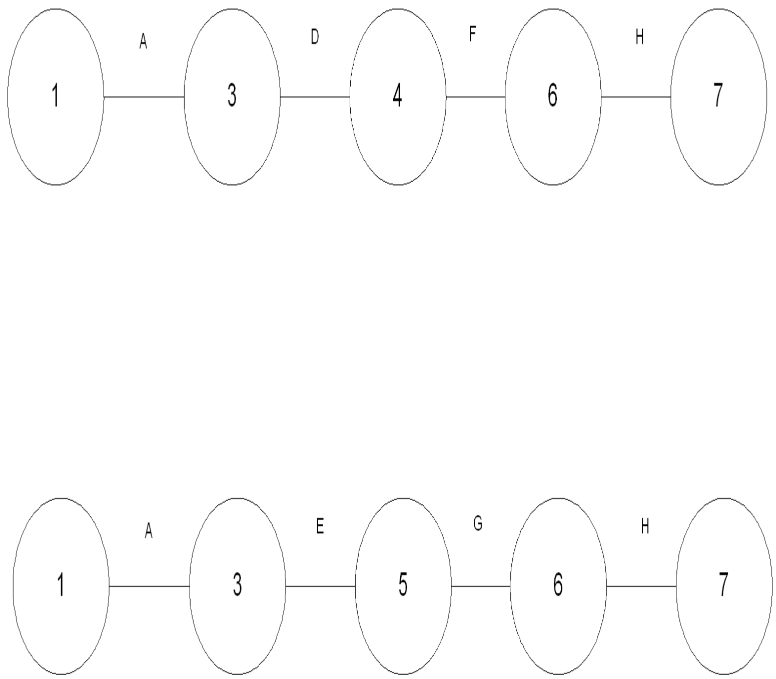

Figure 6.43: Two critical paths.

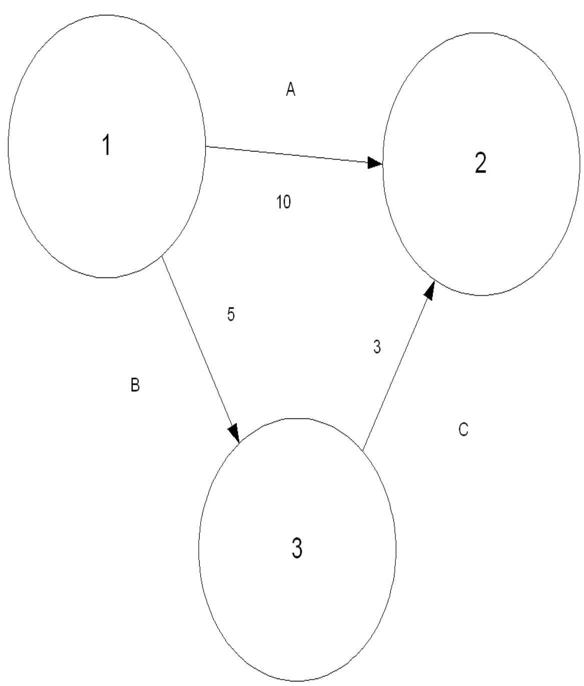

Figure 6.44: Do not crash job A.

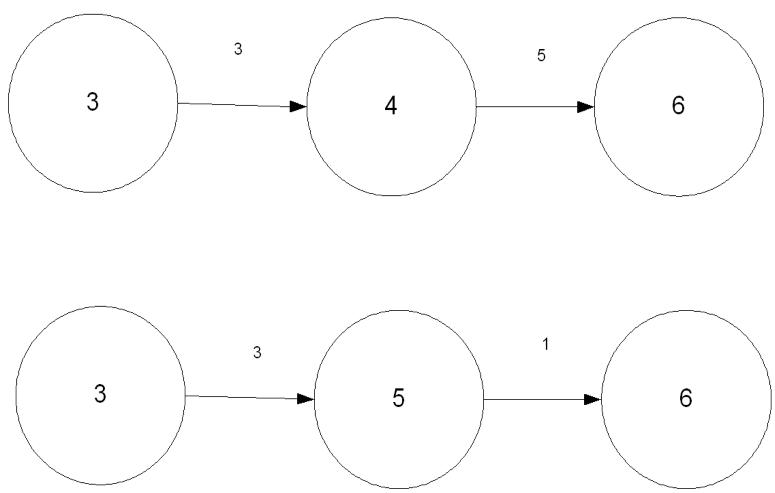

Figure 6.45: Two possible jobs to crash.

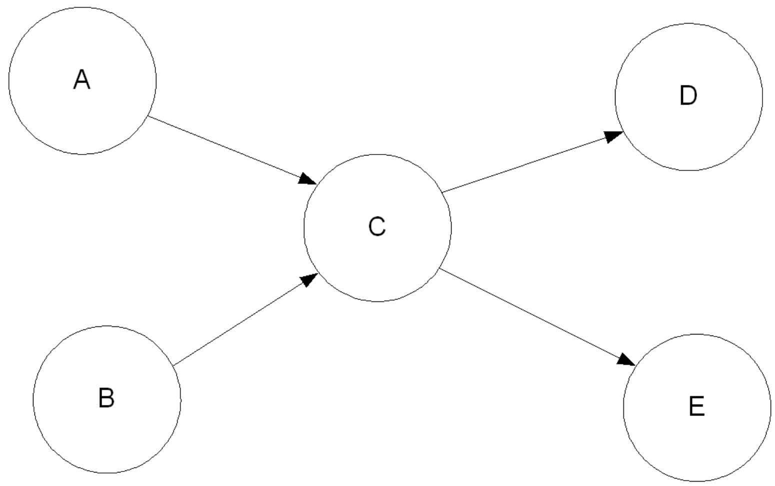

Figure 6.46: Activity on the node example.

Suppose there are significant advantages to having the activities represented as nodes. So, arcs now represent the precedence relationships, and you can omit the dummy arcs — no longer need them. See Figure 6.46.

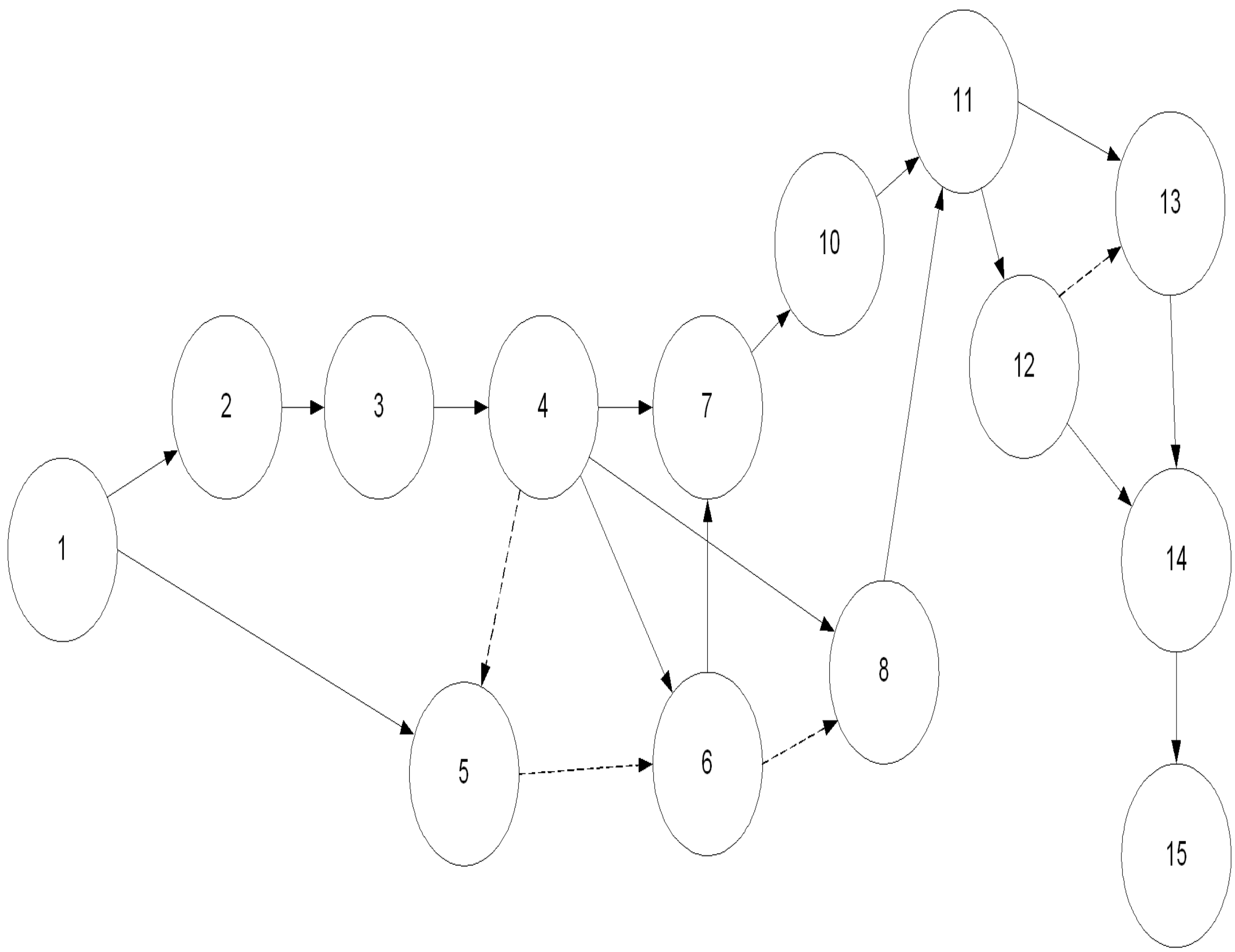

Figure 6.47: The pipe line example with activities on the arcs.

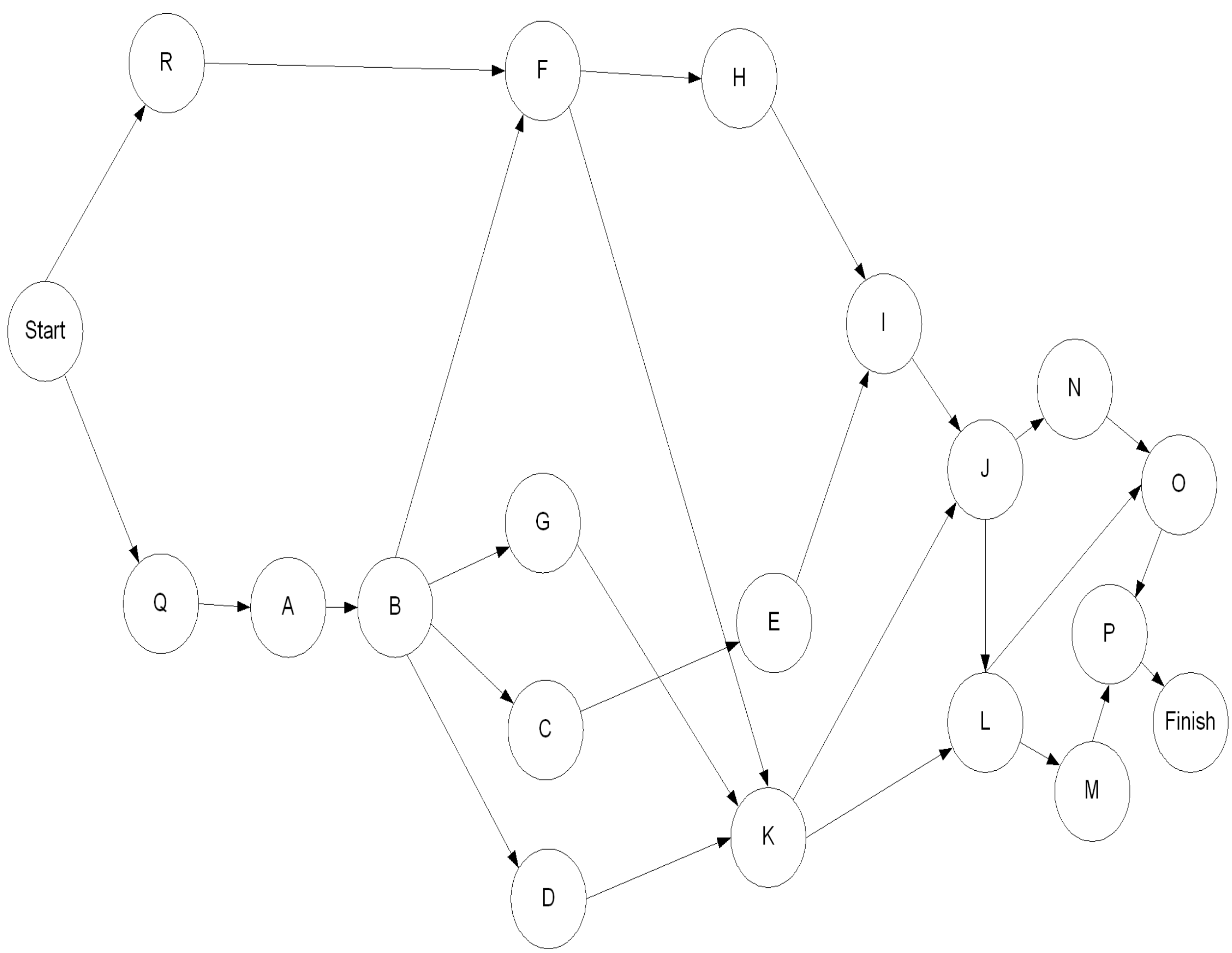

Figure 6.48: The pipe line example with activities on the nodes.

Activities A, and B must preceed activity C. Activity C must preceed D, and activity C must preceed E. Each activity will ha a start time and a finish time. To construct the networks, add a dummy "source" or start and "destination" or finish node.

See page 287 of the text book for the pipeline example;e. In a chemical processing plant, a reactor and storage tank are connected by a 3" insulated process line. Because of erosion, the line needs to be replaced periodically. Along the line, and at the terminal are valves that also need to be replaced. Problems create a time table for periodic maintenance — activities, ordering pipes, give notice of shut down, etc. Figure 6.47 shows the activity on the arc network. Figure 6.48 shows the activity on the node representation.

A note on float: There is an implicit assumption in the total float computation that all of the predecessor activities (at least of these having any relevance to the activity under consideration) must be completed as early as possible; and that all the successor activities are forced to be accomplished as late as possible to realize the total float for one activity. In other words, the total float assumes that no activity takes longer than planned. Hence, in practice, it is generally impossible for each activity to realize it total float since the total float for one activity is closely correlated with the total float of other activities. For example, activity C can exercise its 3 units of total float only by causing activities E, I and J to haven none. Whereas, our float calculations had allocated E, I, and J 3 units of float.

6.7 PERT

The Program Evaluation and Review (PERT) technique is related to the CPM. The CPM includes no notation of probability. It assumes that job times are linear, but can be decreased somewhat at a linear cost. However, in may projects, such as research and development projects, activities have never been done before. Hence, prior experience cannot provide a value for the activities duration. PERT takes explicity account of un-certainties in an activity's duration. For a PERT activity, the user must furnish a most possible time (denoted by M) and an optimistic time (denoted by a), and a pessimistic time (denoted by b). These should be chosen so that the probability that the activities' duration falls outside $[a, b]$ is very small. Consider the beta distribution where $M, \mu \in [a, b]$, and M falls to the left of μ. μ represents the average activity time and may be approximated by

$$\mu = \frac{a + 4M + b}{6}$$

for the beta distribution. The variance of the job time depends on how close a and b are to each other. For most uni-model distributions, the end values lie with in 3 standard deviations from the mean value (as an example, think of the normal distribution). Thus, the spread (or deviation) of the distribution is at 6 times the standard deviation θ. Thus, $6\theta = b - a$ or $\theta = \frac{b-a}{6}$. Thus, $\theta^2 = \left(\frac{b-a}{6}\right)^2$ is the variance of the job time. Thus, PERT requires the activity network and estimates m, a, and b for each activity. Then, the average time μ is found for each activity. Using the average time as actual times, then find the critical path. The duration of the project (T) is the sum of all job times in the critical path. What about the activities that are not on the critical path? You could expect them to overlap with a completely different critical path in the end. This is one of the criticism of PERT. Since the job times themselves are random variables, T is also a random variable. So we can find the mean, μ, and variance θ^2 of T. The expected length of the project is the sum of all the average times of the jobs in the critical path. Similarly, the variance of the project duration is the sum of all the variances of the jobs in the critical path. This assumes independence, which may not always be true. For example, weather affect a lot of activities for a builder — dependence.

Example: Consider a project consisting of 9 jobs (A, B, ..., I) with the following precedence relations and time estimates.

Job	Pred	Opt Time (a)	Most Prob Time (M)	Pessissimistic Time (b)
A	–	2	5	8
B	A	6	9	12
C	A	6	7	8
D	B, C	1	4	7
E	A	8	8	8
F	D, E	5	14	17
G	C	3	12	21
H	F, C	3	6	9
I	H	5	8	11

Using the formulas for μ and θ^2 in the beta distribution, we obtain the following table.

Job	μ	θ	θ^2
A	5	1	1
B	9	1	1
C	7	$\frac{1}{3}$	$\frac{1}{9}$
D	4	1	1
E	8	0	0
F	13	2	4
G	12	3	9
H	6	1	1
I	8	1	1

6.7.1 Critical Path Method

There is a flaw in PERT. Once we have found the CP, we ignore all other paths. It is bad to assume this since we are dealing with averages. There may be a non-CP that has the time close to the critical time, since it's time is probabilistic. It may be in fact completed below the mean time and consequently start it's own CP which we overlooked. Consider the critical jobs A, B, D, F, H, and I in Figure 6.49. Letting T denote the project duration, $E(T)$ is the sum of the expected times on a critical path. $E(T) = 5+9+4+13+6+8 = 45$ days. The variance of the project duration is $Var(T) = 1+1+1+4+1+1 = 9$(add all the CP variances). $\theta(T) = \sqrt{Var(T)} = \sqrt{9} = 3$.

Probabilities of Completing the Project

The project length T is the sum of all the job times on the critical path. PERT assumes that all the job times are iid. Under these assumptions, by the Central Limit Theorem T has a normal distribution with a mean of $E(T)$ and a variance of $Var(T)$.

Central Limit Theorem. Let $x_1, x_2, ..., x_n$ be iid random variables. Then, for large n the sum of the random variables $s_n = x_1 + x_2 + \cdots + x_n$ is normally distributed with a mean $\sum_{i=1}^{n} E(x_i)$ and a variance $\sum_{i=1}^{n} Var(x_i)$. For the PERT method, the independence assumption is shoody enough! And identically distributed is ridiculous! And also, for "large n" means that $n > 30$. Many projects have less than 30 jobs. In our example, T is normally distributed with a mean of 45 and a standard deviation of 3. The assumptions that we have made so far are:

- The activity times have a Beta distribution.
- The activity times are independent.

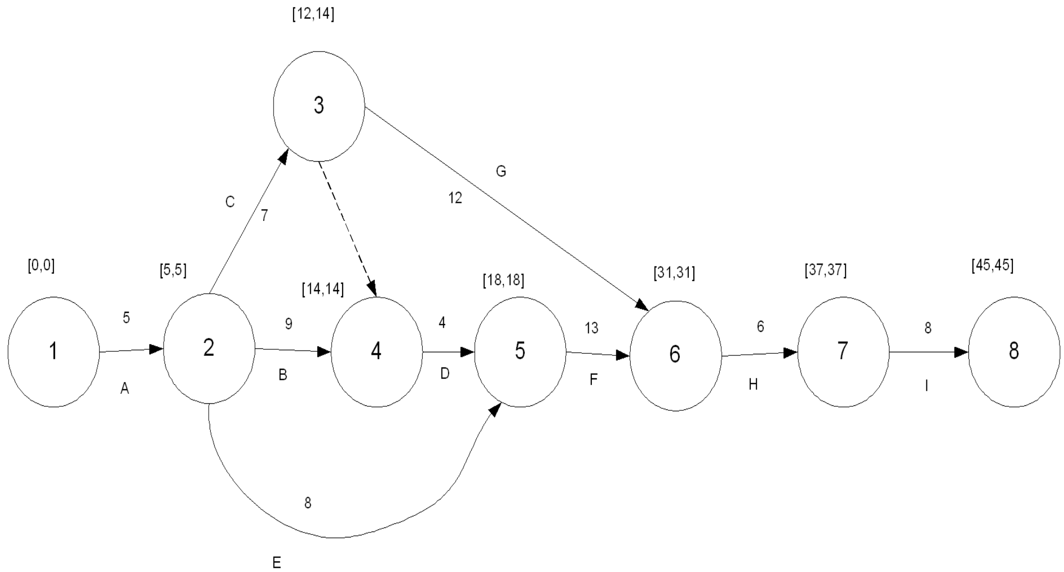

Figure 6.49: The Critical Path Method

- The activity times are identically distributed.
- There are enough activities in the CP that the Central Limit Theorem holds true.
- The CP remains unchanged despite the variability in the activity times.

See Figure 6.50 (note that the curve is not drawn quite right, RLG). Under these assumptions, we can answer some probability questions. For example, for any normal distribution, the probability that the random variable T lies with in one standard deviation from the mean of 0.68. There is a 68% chance that the project duration will lie with in [42, 48]. Similarly, there is a 99% chance that T will lie with in 3θ, i.e. 36 and 54.

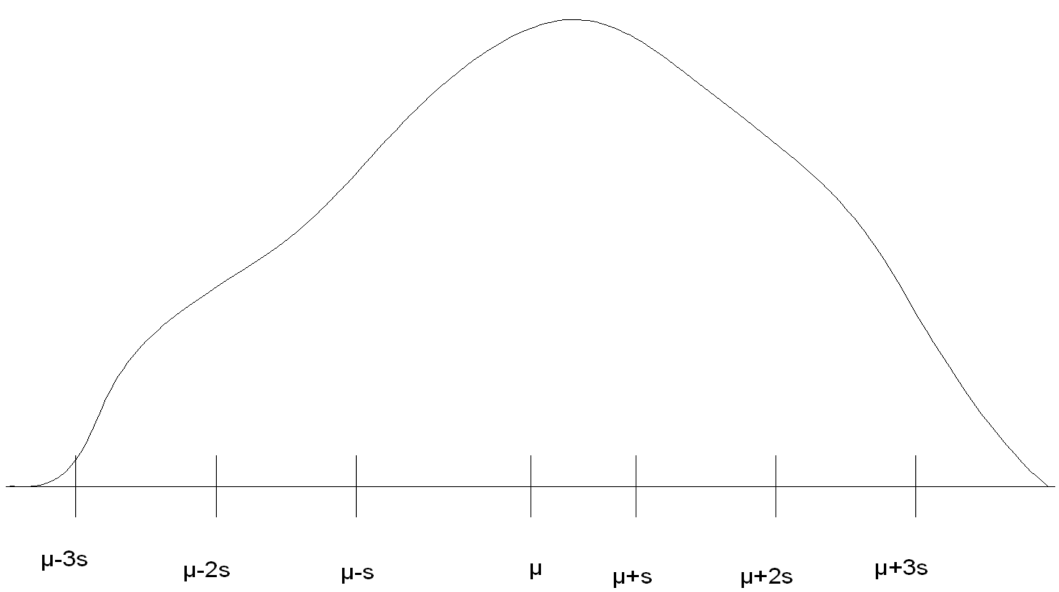

Figure 6.50: The normal distribution (note curve is not as symmetric as it should be).

We can calculate the probabilities of meeting specific deadlines. For example, $P(T \leq 50), T \sim N(45, 9)$. Letting $z = \frac{T-E(T)}{\sigma(T)}, z \sim N(0,1)$. Then,

$$P(T \leq 50) = P\left(z \leq \frac{50-45}{3}\right) = P(z \leq 1.67) = 0.95.$$

$$P(T \leq 41) = P\left(z \leq \frac{41-45}{3}\right) = P(z \leq -1.33) = 0.09.$$

So the chance of completing the project four days early is 9%.

6.7.2 Difficulties with PERT

Some of the difficulties with PERT include:

- Activity durations are not really iid.
- Activity durations may not follow the beta distribution.
- The assumption that the CP found by CPM will always be the critical path for a project may not be justified. (This is a serious difficulty).

See Figure 6.51 for this example.

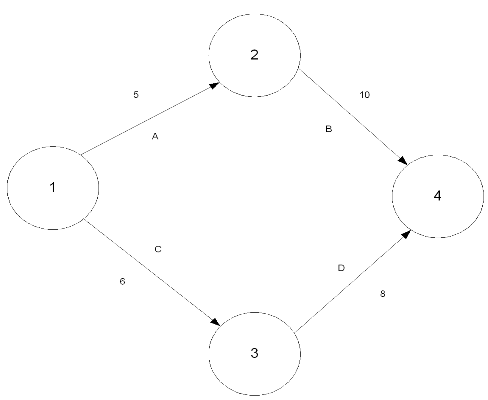

Figure 6.51: An example of a PERT model

	a	b	m
A	1	9	5
B	6	14	10
C	5	7	6
D	7	9	8

There is more variability with A and B, and less variability with C and D. So in reality, we could have C is 6, D is 8, A is 4, and B is 9. Then, $C + D = 14$, and $A + B = 13$ A and B is not the critical path anymore. If we assume that the durations of the paths are independent random variables, then it can be shown that there is a chance that A and B is not a critical path.

Path	Probability Being Critical
A, B	$\frac{10}{27}$
C, D	$\frac{15}{27}$
A, B and C, D	$\frac{2}{27}$

The probabilities that an activity will be critical are given in the following table.

Activity	Probability
A	$\frac{17}{27}$
B	$\frac{17}{27}$
C	$\frac{12}{27}$
D	$\frac{12}{27}$

6.7.3 Alternative to PERT

One can use Monte Carlo simulation. In this alternative, we can drop all of those unrealistic assumptions. Up to now, for generalized networks, we have assumed that:

1. All activities preceeding an event must be completed before any activities emulating fro the event could be performed.
2. All activities in the project must be performed.

But sometimes we want to model a situation where any of a number of activities is sufficient to begin the next activity. Some examples of where (1) does not hold are:

- Any one of several causes is the prerequisite for another cause.
- Arrival of any of a number of expected checks (paycheck, box check, etc) will enable you to begin shopping.
- Success of any one of the several grant proposals would suffice to finance a research project.

Some examples of where item (2) in the generalized project network list does not hold true include:

- Elective courses in the curriculum.
- A milling job may have to go through 1, 2, or 3 drilling's depending on the result of the quality controls.
- The choice of advertising depends on the results of the surveys.

Generalized networks allow these problems to be modeled. Project networks have only one type of vertex, *event vertices.* Generalized networks have several types of vertices called *decision boxes.* There are three different conditions can be placed on the activities entering the decision box.

1. 'AND' Input: all activities entering the decision box must be performed before the decision box is considered completed.
2. Inclusive Input: at least one activity entering the decision box must be performed before the decision box is considered complete.
3. Exclusive Input: exactly one of the activities entering the decision box must be performed before the decision box is considered complete.

In addition, two different conditions can be placed on the activities' emulating from a decision box.

1. Deterministic Output: all activities emulating from the decision box are to be performed once the decision box has been completed.
2. Probabilistic Output: exactly one of the activities emulating from the decision box is performed after the decision box has been completed, according to a probability distribution.

So, there are $3 \times 2 = 6$ shapes in the network instead of just the O's with PERT and CPM. See Figure 6.52.

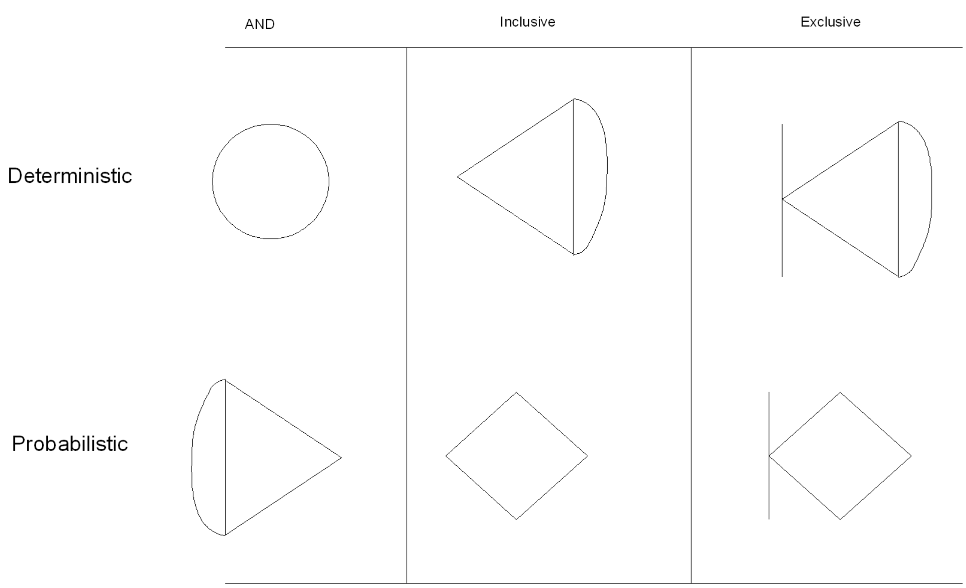

Figure 6.52: Shapes used in generalized networks.

Basically, the input is the first half of the symbol, and the output is the second half of the symbol. So, 'AND' is denoted by $(,)$ and is deterministic. Inclusion is denoted by $<,>$ and is probabilistic. Exclusion is denoted by $| <$. Put those three symbols together in all combinations and you will get the six symbols in Figure 6.52.

In a project network, a time $t(x, y)$ was specified for each activity (x, y). In a generalized activity network, both a time $t(x, y)$ and a probability $p(x, y)$ must be specified for each activity (x, y). $p(x, y)$ is the probability that activity (x, y) will actually be performed once the decision box x has been reached. If the decision box x has a deterministic output, then $p(x, y)$ must equal to 1 and the activity $x, y)$ is certainly performed. Moreover, the sum of the probabilities of the activities emanating from a probabilistic decision box must

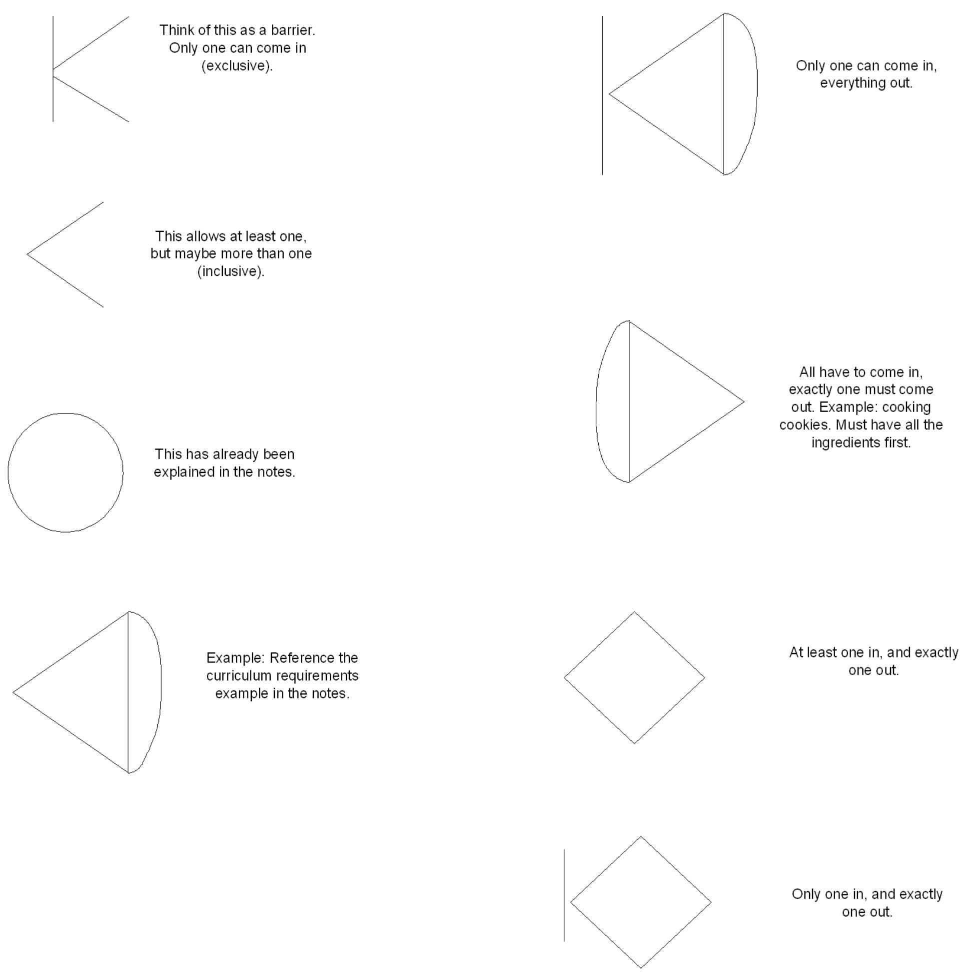

Figure 6.53: Examples

equal 1.

Example: Consider the network in Figure 6.54. On some generalized project networks, you always finish the project! Consider arcs $(2,5)$ and $(3,5)$. We will skip node 4, but that's ok! Not all nodes are passed through. Not that you can never get to node 5. For another example, we may never get past node 4 because $(2,4)$ and $(3,4)$ both cannot go into node 4.

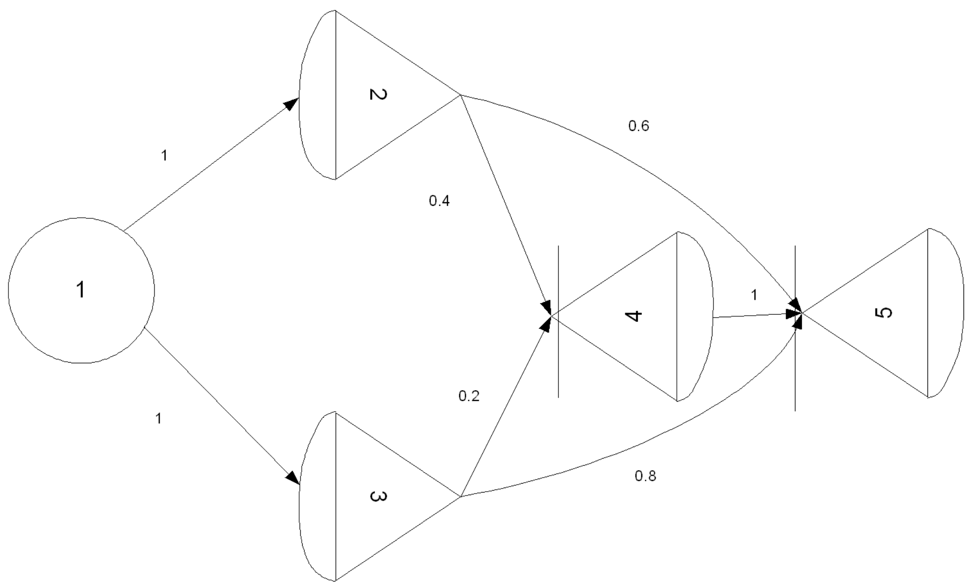

Figure 6.54: Example of a generalized project network.

Example: A journal welcomes contributions from would-be authors. Upon receipt of a manuscript, the magazine simultaneously submits it to two referees. A referee may say "reject," "accept" or "undecided" with respective probabilities 0.50, 0.40 and 0.10. If at least one referee says "reject" then the manuscript is rejected. If both referees say "accept" then the manuscript is accepted. Otherwise the article is sent to a third referee. See Figure 6.55. One variation of the above example supposes that the editor does not send the manuscript to the second referee unless the first referee thinks an acceptance or undecided verdict will result.

In a project network, all events are eventually reached — it is merely a matter of time. The same is not necessarily true for a generalized project network. In our example, observe either accept, reject, or the third referee will be reached. It can also happen that the project will terminate, not with a decision box, but with an activity. For example, in our simplest general network, if both (2,4) and (3,4) are performed, then the project ends without reaching decision box 4. However, this can occur only if exclusive input decision box's are present in the network.

In a generalized project network, not all arcs will be traveled and there may be a variety of possible terminal nodes. The project manager will want to know the probability that any decision box will in fact be reached and that any activity will in fact be performed. Moreover we wish to know the expected time at which a decision box will be reached (if it is reached at all).

Contrast with PERT: In PERT, the actual time is required to perform an activity was random. But, we were certain that the activity would sooner or later be performed. In a generalized network, the opposite occurs. The time required to perform an activity is assumed to be a known constant, but the activities that are performed are randomly selected.

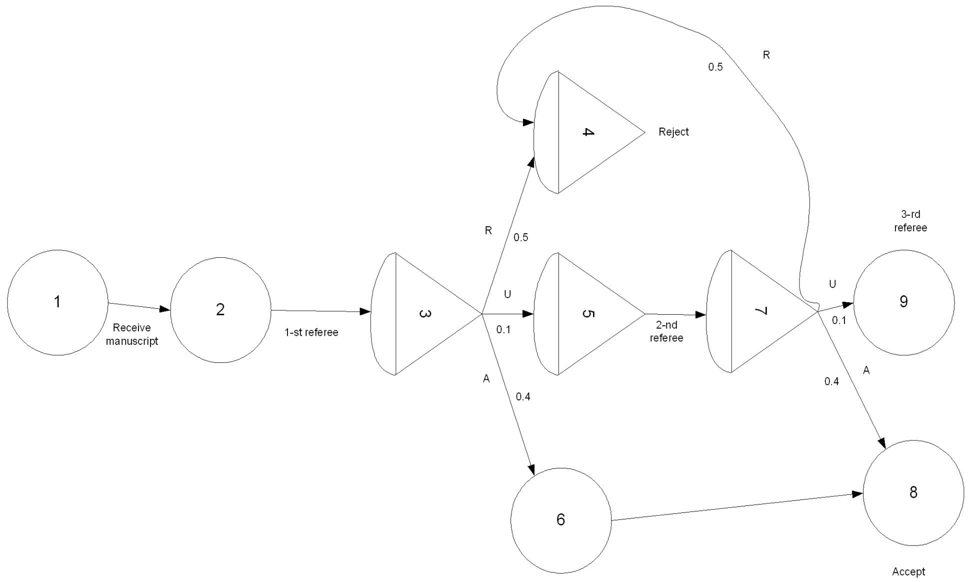

Figure 6.55: Example of the referee problem.

6.7.4 Solving a Generalized Network

These problems and expected times are not easy to calculate. The difficulty is because of the presence of probabilistic decision boxes. Only one of the set of activities emulating from a probabilistic output decision box may occur. Hence, the probabilities of actually completing activities and decision boxes following a probabilistic output decision box are not statistically independent. Therefore, we cannot use the usual probability rules.

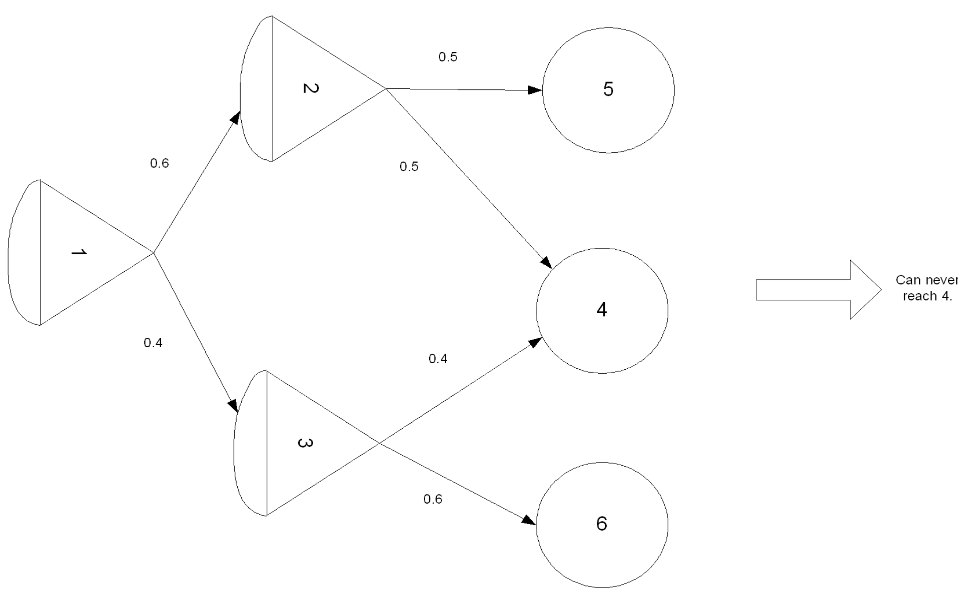

Figure 6.56: The generalized network where node 4 is never reached.

For example, consider the generalized network in Figure 6.56. We can never reach node 4, because only one path comes out of decision box 1. Both activities (2,4) and (3,4) must be performed before decision box 4 is reached. There is a $0.60 \times 0.50 = 0.30$ probability that (2,4) is performed. There is a $0.40 \times 0.40 = 0.16$

probability that (3,4) is performed. So what is the probability that decision box 4 is reached? It's not $0.30 + 0.16$ because if two events are statistically independent, knowing that one has occured does not change the probability that the other has occurred. So, $P(A|B) = P(A)$ and $P(A \cap B) = P(A)P(B)$. But, we do not have statistical independence here! The lack of statistical independence for activity probabilities leaves large networks virtually untraceable. Even if the definition of the probabilistic output decision box were changed so that any number of activities could emanate from it, the same computational difficulties would arise. Another serious difficulty is the presence of cycles. For example, an activity might have to be repeated until it is performed correctly. Such as a required course in a university program. Thus, the calculations become even more complex.

6.7.5 Complex GPN Calculations

How do we deal with GPN when the calculations become complex?

1. Use Markov chain networks. See Figure 6.57.

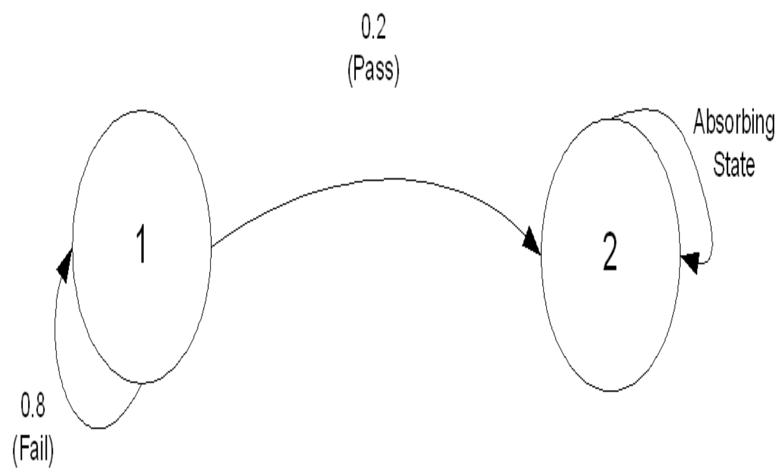

Figure 6.57: Markov chain example.

2. Use simulation.

6.8 Homework and Answers

There are 100 points in this problem set. Do your own work without consulting with others. Careful partial credit will be given — show all work except trivial arithmetic.

1. Find the minimum cost production schedule to meet demands in the next 4 periods. Draw a shortest path network and solve using Dijkstra's algorithm.

Period	1	2	3	4
Set-up	50	100	50	70
Demand	60	100	140	200
Unit prod. cost	7	7	8	7
Unit hold. cost	1	1	2	2

The cost of *successive periods* is calculated as follow:

$$C_{ij} = D_i P_i + S_i.$$

Notice there is no holding cost in that equation. Holding costs occur when demand is satisfied by producing in a previous period. As an example, suppose demand is met in periods 1, 2, 3 by producing everything in period 1. Then, the cost is calculated as follow:

$$C_{14} = S_i + P_i(D_1 + D_2 + D_3) + H_i(D_2 + D_3) + H_{i+1}(D_3) =$$

$$50(7)(300) + 1(240) + 1(140) = 2530.$$

Other costs are obtained in a similar way.

In the network diagram, let each node represent a period. Let each arc represent the cost C_{ij} from going from node i to node j. Applying Dijkstra's algorithm results in a minimum cost of \$3860. The optimal path thru the network is $1 \to 2 \to 4 \to t$. It makes sense that period 3 has been left out of the minimum path. There is a higher production cost in period 3. It is more economical to produce the demand in period 3 in period 2. Note that the holding cost in period 4 was never used since we had no information about demand in period 5. A trace follows.

Step 1:

$$d(1) = 0; d(i) = \infty, i = 1, ..., 4, t.$$

Step 2:

$$d(2) = \min(\infty, 470) = 470.$$

$$d(3) = \min(\infty, 1270) = 1270.$$

$$d(4) = \min(\infty, 2530) = 2530.$$

$$d(t) = \min(\infty, 4730) = 4730.$$

Therefore, make $d(2)$ permanent.

$$d(3) = \min(1270, 470 + 800) = 1270.$$

$$d(4) = \min(2530, 470 + 1920) = 2390.$$

$$d(t) = \min(4730, 470 + 3920) = 4390.$$

Therefore, make $d(3)$ permanent.

$$d(4) = \min(2390, 1270 + 1170) = 2390.$$

$$d(t) = \min(4390, 2390 + 1470) = 3860.$$

Therefore make $d(4)$ permanent and make $d(t)$ permanent.

2. Suppose a message is to be sent between two nodes of a communication network. Assume that the individual communication links(edges) operate independently with a known set of probabilities. What path between the two nodes has the maximum reliability, that is, probability that all of its edges are operative? Show how to formulate this problem as a shortest path problem and apply it to the following network(careful, shortest route problem minimizes a sum). See Figure 6.58.

What if the numbers on the arcs had represented probability of failure instead of probability of successful transmission? Explain how this will change the problem solution method.

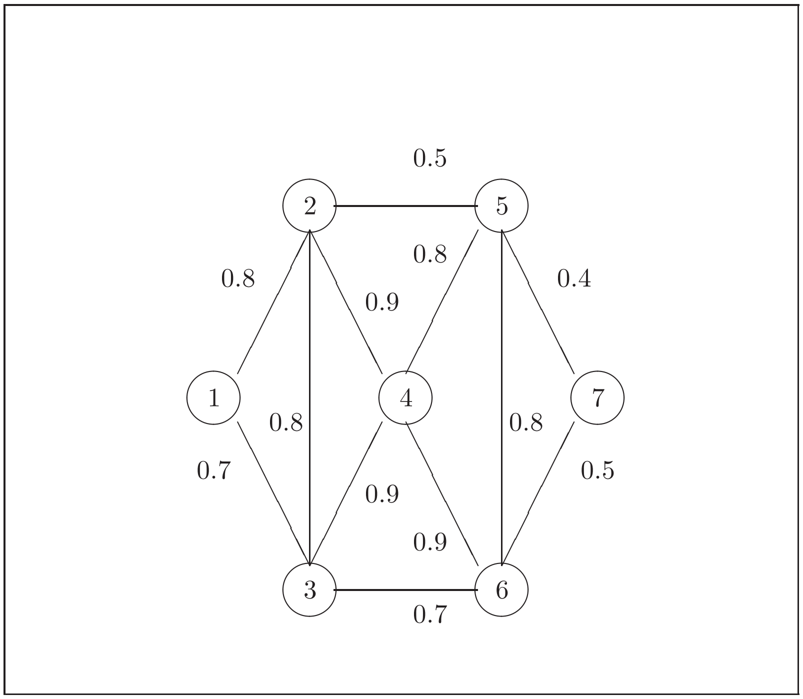

Figure 6.58: Communication Network

3. See Figure 6.59. A hotel manager must make reservations for the bridal suite for the coming month. The hotel has received a variety of reservation request's for various combinations of arrival and departure days. Each reservation would earn a different amount of revenue for the hotel due to a variety of rates for students, employees, airline personnel, etc. How can the Dijkstra algorithm be used to find the best way to schedule the bridal suite with maximum profits to the hotel?

   Draw a network for the month of June. Explain what the nodes represent and what the costs are and how they are computed. Make up a simple numerical example for the first 4 days of June to illustrate the idea.

   - A hotel manager receives request's for reservations of the bridal suite for the coming month. The reservations are varied with different combinations of arrival and departure days. Each reservation would earn a different amount of revenue for the hotel due to a variety of rates for students, employees, airline personnel, etc. How can Dijkstra's algorithm be used to find the best way to schedule the bridal suite i-th maximum profits to the hotel?

     Each node n has $n-1$ arcs coming into it. Each node represents a day in June, while each arc (i, j) represents the profit made by the hotel for a person staying in the bridal suite arriving day i and leaving day j. This is why each node n has $n-1$ arcs coming into it, to incorporate all possible reservation patterns. Also, the first day of July must be included in the network because allowances have to be made for someone staying thru the last day(i.e. leaving on the first day of July). This would still count in June's figures. That node also allows for someone to arrive on the 30-th of June and leave the next day, which is relevant for June's reservations, not July's.

     Cost presentation: Each arc (i, j) represents the best(i.e. the maximum) profit available to the hotel of all reservations in which arrivals occur on day i and departures on day j. $Profit = Revenue - Costs$. Total Revenue is the room rate multiplied by the number of nights staying. Then, total costs are (room rate times applicable discount plus operating costs) times the number of nights staying. Therefore, profit for arriving on day i and departing on day j is

$$P_{ij} = R_{ij} - c_{ij} = r_{ij}(j-1) - (r_{ij}d_\alpha + k_{ij})(j-i) = (j-i)[r_{ij} - r_{ij}d_\alpha - k_{ij}].$$

- The table below is a list of the reservation request's for the first 4 days.

By Whom	1-2	1-3	1-4	1-5	2-3	2-4	2-5	3-4	3-5	4-5
Business	1	0	0	0	1	1	0	0	0	0
Student	1	1	0	0	0	1	0	1	1	0
Employee	0	1	1	0	0	0	0	0	0	1

Let the regular room rate be \$100 per night with a constant operating cost of \$1 per night. The discounts are 10% for students, 7% for employees, and 5% for businesses. According to the requested reservations, room rates, and discounts, the profit table looks like the following:

By Whom	1-2	1-3	1-4	1-5	2-3	2-4	2-5	3-4	3-5	4-5
Business	\$94	0	0	0	\$94	\$188	0	0	0	0
Student	\$89	\$178	0	0	0	\$178	0	\$89	\$178	0
Employee	0	\$184	\$276	0	0	0	0	0	0	\$92
Column Max	\$94	\$184	\$276	0	\$94	\$188	0	\$89	\$178	\$92

Choose the maximum possible profit for staying from day i to day j to be the arc profit for (i, j). To find the reservation schedule that will maximize profit, use Dijkstra's algorithm. However, the arc costs must be adjusted in order to minimize in Dijkstra's algorithm. Since 276 is the largest arc cost, subtract all the remaining arc costs from that and relabel the network.

Step/Node	1	2	3	4	5
0	0	∞	∞	∞	∞
1	0	182	92	0	276
2	0	182	92	0	184
3	0	182	92	0	184
4	0	182	92	0	184

- The path that yields the minimum cost of the altered network is found by working backwards thru the network. Arc (i, j) is the path if $\gamma_j = \gamma_i + c_{ij}$. So, from 5 to 4:

$$\delta_4 + c_{45} = 0 + 184 = \delta_5.$$

$$\delta_3 + c_{35} = 92 + 98 \neq \delta_5.$$

$$\delta_2 + c_{25} = 182 + 276 \neq \delta_5.$$

$$\delta_1 + c_{15} = 0 + 276 \neq \delta_5.$$

From 5 to 4 to 1:

$$\delta_3 + c_{34} = 92 + 187 \neq \delta_4.$$

$$\delta_2 + c_{24} = 182 + 88 \neq \delta_4.$$

$$\delta_1 + c_{14} = 0 + 0 = 0 = \delta_4.$$

According to Dijkstra's algorithm, the shortest path thru the network is 1 to 4 to 5. This yields a profit of $\$276 + \$92 = \$368$. This answer can be interpreted in the following manner: the hotel manager should rent the room to employee #1 who requested to stay from day 1 to day 4 with a profit of \$276. Then, the hotel manager should rent the room to employee #2 who requested to stay from day 4 to day 5 with a profit of \$92. This schedule yields a total profit of \$368.

NOTE: Just by looking at the network, it seems that a better, more profitable solution would be the path 1–2–4–5, which yields a profit of \$374. I have tried to determine the error in my formulation, but I don't really know why it did not work...Paige Burger.

4. Consider the following network in Figure 6.59:

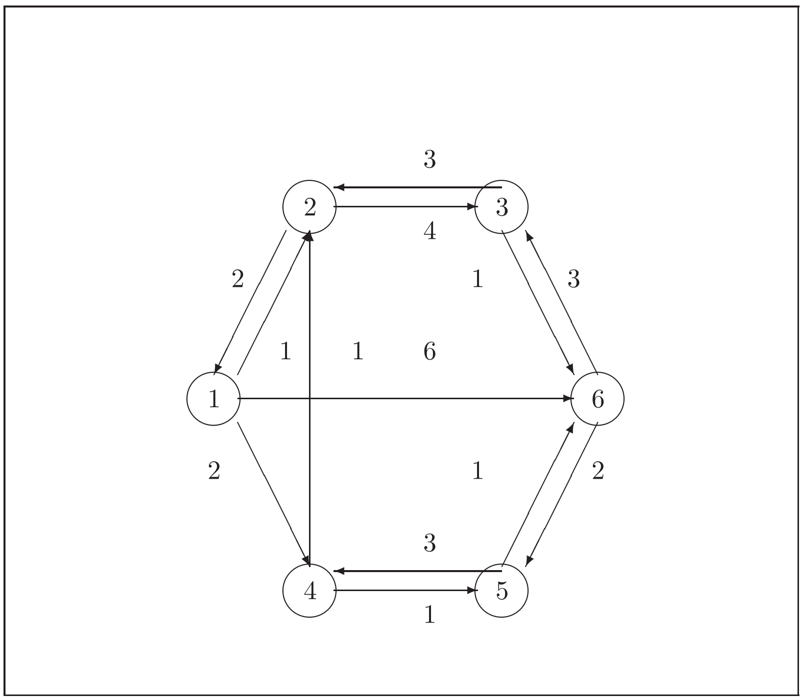

Figure 6.59: A Network

Find the minimum cost path from 1 to 6 using Dijkstra's algorithm.

5. Problem 6, p385 in Hillier and Lieberman. HINT: Let node (i, j) denote phase i being completed with j left to spend. You will have 3 nodes for phase I, i.e. (1,27), (1,24), and (1,21), depending on your decision of how much to spend. On phases 2 thru 4, there will be 4 nodes for each phase, for a total of 17 nodes including a beginning (0,30) node and a terminal node T. Arc costs are $t_{(i,j),(i+1,k)}$ representing the time taken to complete phase $i+1$ if $(j-k)$ million dollars is spent. This data is in the table.

Solution: In this problem we were asked to minimize the time needed to complete the development of a new product in 4 non-overlapping phases. We were given a budget of \$30 million to complete the 4 phases. Each node in the network corresponds to money left over after spending money in a particular phase. The arcs represent times needed to complete a phase at a certain pace. There are 3 paces of work that could be completed. 1) normal, 2) priority, and 3) crash. A crash pace is usually the fastest but requires the most money. We are asked in the problem to apply the algorithm in Section 10.3 of the Hillier book. The algorithm sounded like Dijkstra's algorithm. Only the authors forgot to mention marking all the nodes with infinity. So, I decided to apply Dijkstra's algorithm as we know it. The results are on the next few pages. See Figure 6.60 and Figure 6.61.

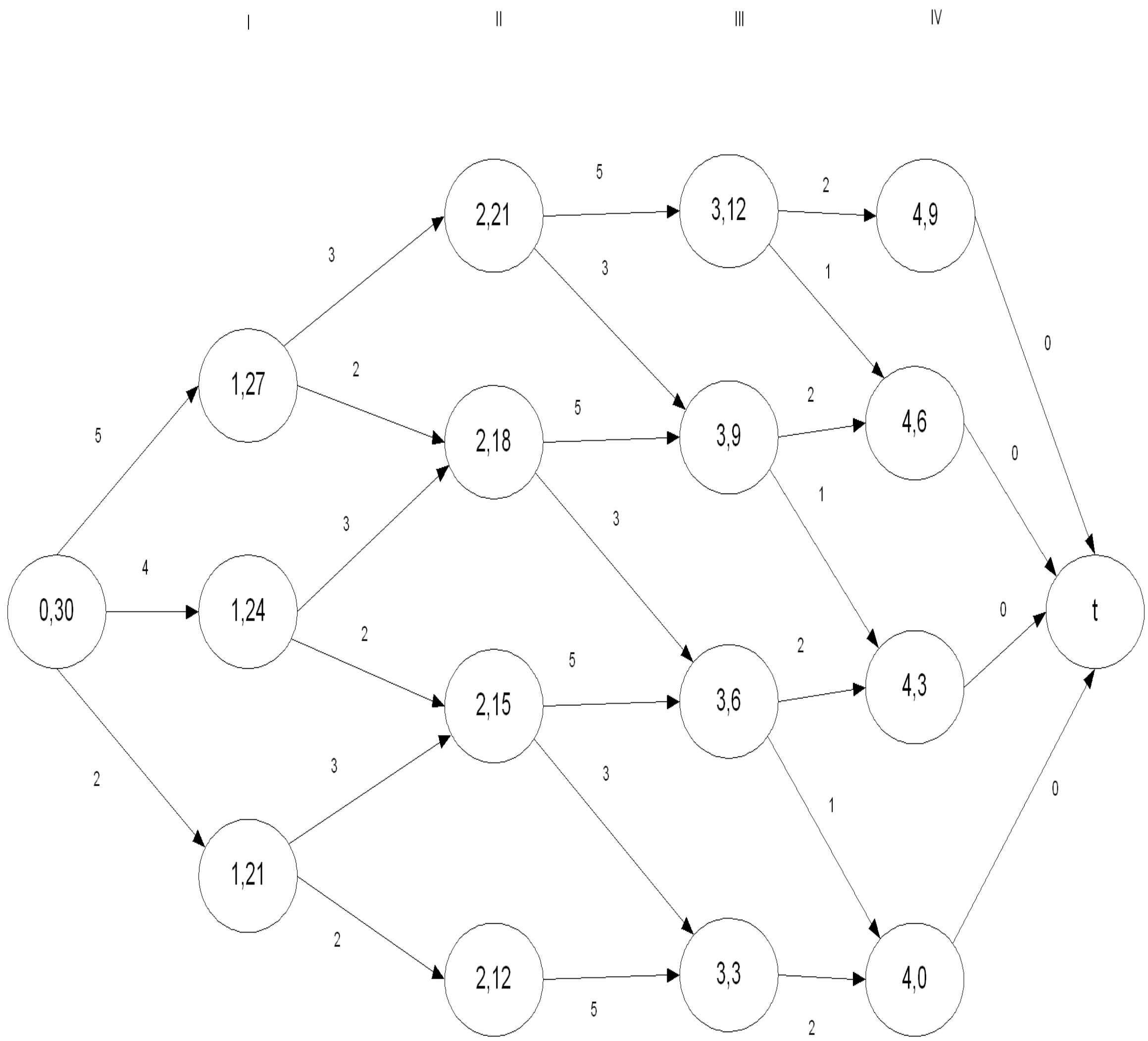

Figure 6.60: The network showing the 4 phases of the problem.

Step 1: $d(1) = 0, d(i) = \infty, i \in N$.

Step 2:

$$d(1,21) = \min(\infty, 2) = 2,$$

$$d(1,24) = \min(\infty, 4) = 4,$$

$$d(1,27) = \min(\infty, 5) = 5.$$

Therefore, make $d(1,21)$ permanent.

$$d(2,15) = \min(\infty, 2+3) = 5,$$

$$d(2,12) = \min(\infty, 2+2) = 4.$$

Therefore, make $d(2,12)$ permanent. Therefore, make $d(1,24)$ permanent.

$$d(2,18) = \min(\infty, 4+3) = 7,$$

$$d(2,15) = \min(5, 4+2) = 5,$$

$$d(3,3) = \min(\infty, 4+5) = 9.$$

Therefore, make $(2,15)$ permanent and make $(1,27)$ permanent.

$$d(2,21) = \min(\infty, 8) = 8,$$

$$d(2,18) = \min(7, 5+2) = 7,$$

$$d(3,6) = \min(\infty, 5+5) = 10,$$

$$d(3,3) = \min(9, 5+3) = 8.$$

Therefore, make $(2,18)$ permanent.

$$d(3,9) = \min(\infty, 7+5) = 12,$$

$$d(3,6) = \min(10, 7+3) = 10.$$

Therefore, make $(d(3,6)$ and $d(4,0)$ permanent.

$$d(t) = \min(\infty, 10+0) = 10,$$

$$d(4,3) = \min(\infty, 10+2) = 12.$$

Therefore, make $d(t)$ permanent.

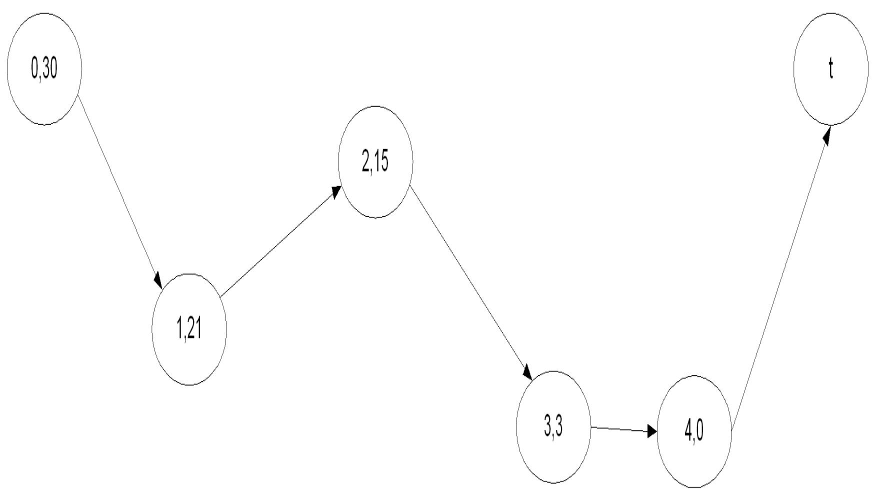

Figure 6.61: The solution to the network with the 4 phases of the problem.

The minimal path is given in Figure 6.61. The total minimum time is 10 at a cost of \$30 million. The optimal policy to pursue, within budget, would be to do work at the crash pace in phase I, a priority pace in phase II and a crash pace in phases III and IV.

6. In the communication network seen in Figure 6.62, the number adjacent to each node indicates the average delay in sending a message on any arc leaving the node. The time required for a message to traverse any arc is essentially zero. Use Dijkstra's algorithm to find the minimum time path for node 1 to node 7.

Solution: In this problem we are given a communication network and asked to find the shortest path using Dijkstra's algorithm. The cost (time) of traversing a node is computed when the message leaves that node. There is essentially no cost of traversing an arc. The shortest path represents the minimal time to send a message through the network. The following list is a trace of Dijkstra's algorithm.

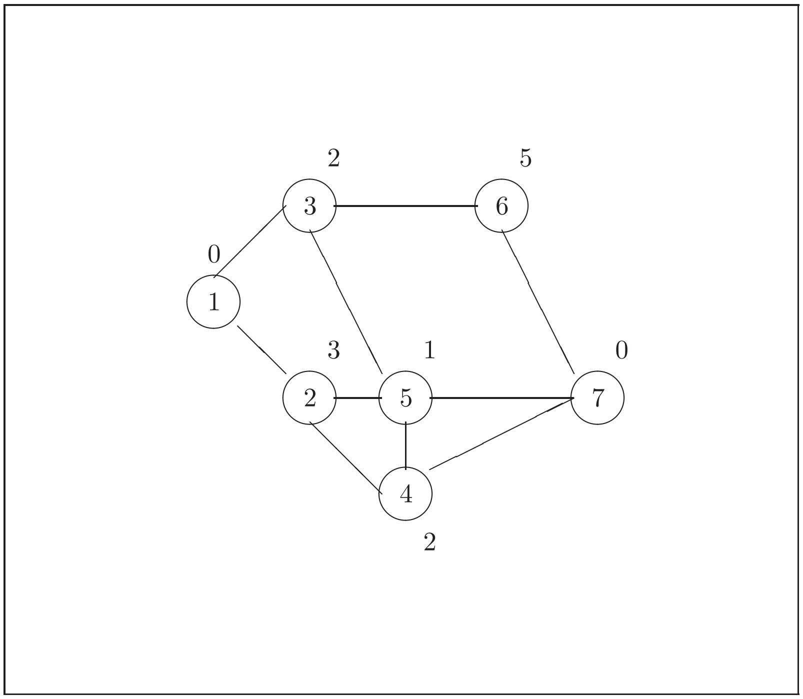

Figure 6.62: Communication Network

Step 1: $d(1) = 0, d(i) = \infty, i = 2, 3, ..., 7.$

Step 2:

$$d(2) = \min\{\infty, 3\} = 3,$$

$$d(3) = \min\{\infty, 2\} = 2.$$

Make $d(3)$ permanent.

$$d(6) = \min\{\infty, 2 + 5\} = 7,$$

$$d(5) = \min\{\infty, 3\} = 3.$$

Make $d(2)$ permanent.

$$d(5) = \min\{3, 4\} = 3,$$

$$d(4) = \min\{\infty, 3 + 2\} = 5.$$

Make $d(5)$ permanent.

$$d(7) = \min\{\infty, 3 + 0\} = 3.$$

Make $d(7)$ permanent. See Figure 6.63.

Therefore, the minimum path from node 1 to node 7 is $2 + 1 + 0 = 3$.

7. Routing of traffic often includes delays at intersections or "turn penalties." For example, in the network in Figure 6.64, every turn incurs a penalty of 3 in addition to the travel times on the arc.

Solve as a shortest route problem.

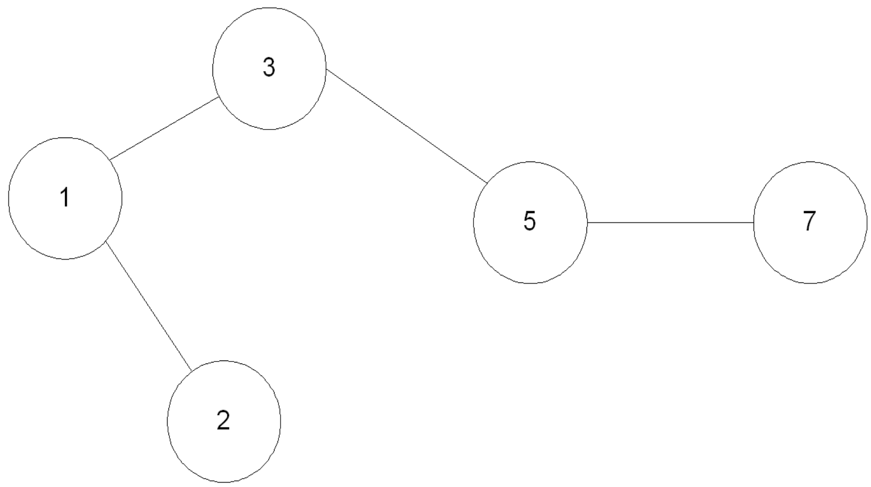

Figure 6.63: The solution to the communications network problem.

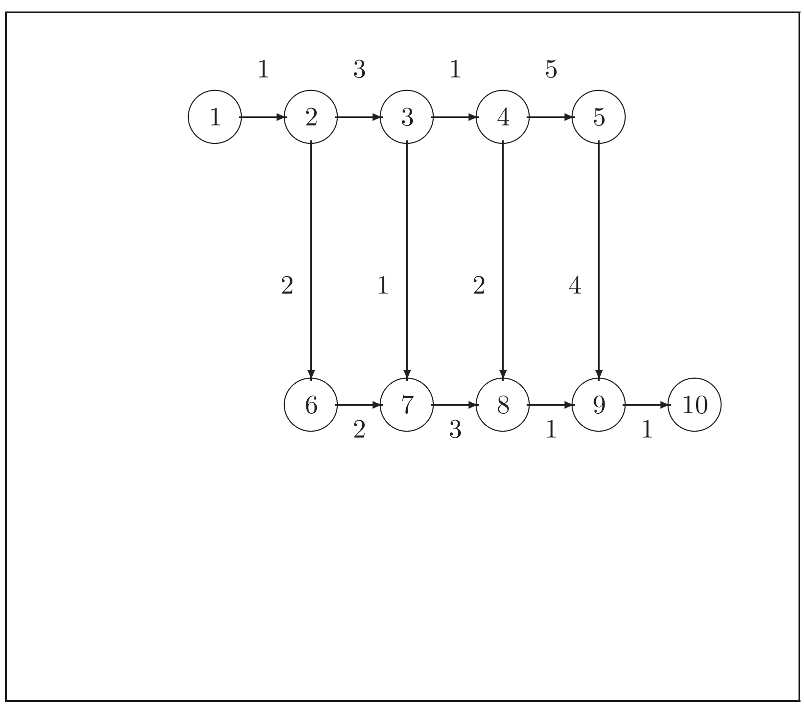

Figure 6.64: Traffic Flow

8. Let the numbers on the network in problem 2 represent distances rather than probabilities and find the minimum spanning tree.

   In this problem, we were given the network diagram in Question 2 and asked to find the minimal spanning tree. The arcs in the graph represent distances. To find the MST, we can start at any node. Simply choose the smallest arc incident to the chosen node. Every time a node is added to the MST, follow the same procedure for the other known nodes by choosing the smallest distance. The procedure stops when every node in the network is in the MST. The trace of the procedure: 1–3, 1–3–6, 1–3–6–7, 1–3–6–7–5, 1–3–6–7–5–2, 1–3–6–7–5–2 and 5–4. The minimal spanning tree is the sum of $0.7 + 0.7 + 0.5 + 0.4 + 0.5 + 0.8 = 3.6$

6.9 Maximum Flow Problems

1. Site selection. See Figure 6.10 on page 326. Select sites for an electronic message transmission system. The costs c_i of establishing site i and revenue r_{ij} if i, j are both selected. The objective is to select sites to maximize net profits. How can we model this as a max flow problem? How can we include fixed costs on the network? When the network flow is reconfigured, to maximize net profits, we need to find the minimum capacity cut between s and t. See Figure 6.65.

2. Computer wiring. A computer interface consists of several modules. On each module are located several pins. A given subset of pins has to be interconnected by wires. Because of the possible modifications and corrections and of the small size of the pin, at most 2 wires can be attached to any pin. In order to avoid signal cross talk and to improve the ease and neatness of wire ability, the total wire length must be minimized.

3. Circuit board drilling. Metalica is a Greek manufacturer of printer circuit boards(PCB). Holes must be drilled in the PCB's at locations that correspond to pins where electronic components will later be soldered on the board. A typical PCB might have 500 pin placements. Most of the drilling is performed by programmable machines. Finding the optimal drilling sequence is a TSP(traveling salesman problem). By solving TSP problems for PCB's on a personal computer, Metalica reduced the time required to drill boards by 30%.

4. Order picking in a warehouse.

6.9.1 Branch and Bound

Example: A symmetric matrix problem.

	1	2	3	4	5
1	—	3	7	6	2
2	4	—	11	9	6
3	3	6	—	1	5
4	5	5	3	—	4
5	6	2	7	6	—

1–3–4–5–2–1 with a distance of 18 is the answer. Greedy heuristic $(1, 5), (5, 2), (2, 4), (4, 3), (3, 1) = 19$. $z^* \leq 19$, z^* is optimal. The lower bound(but not optimal) is found by MST on a symmetric matrix. The general idea of branch and bound:

1. Solve a relaxation of the TSP. If solution is a feasible tour, stop. It must be optimal. If solution is not a tour, then it is a lower bound. At least one of the arcs in this solution which cause the in-feasibility cannot be included in the optimal solution.

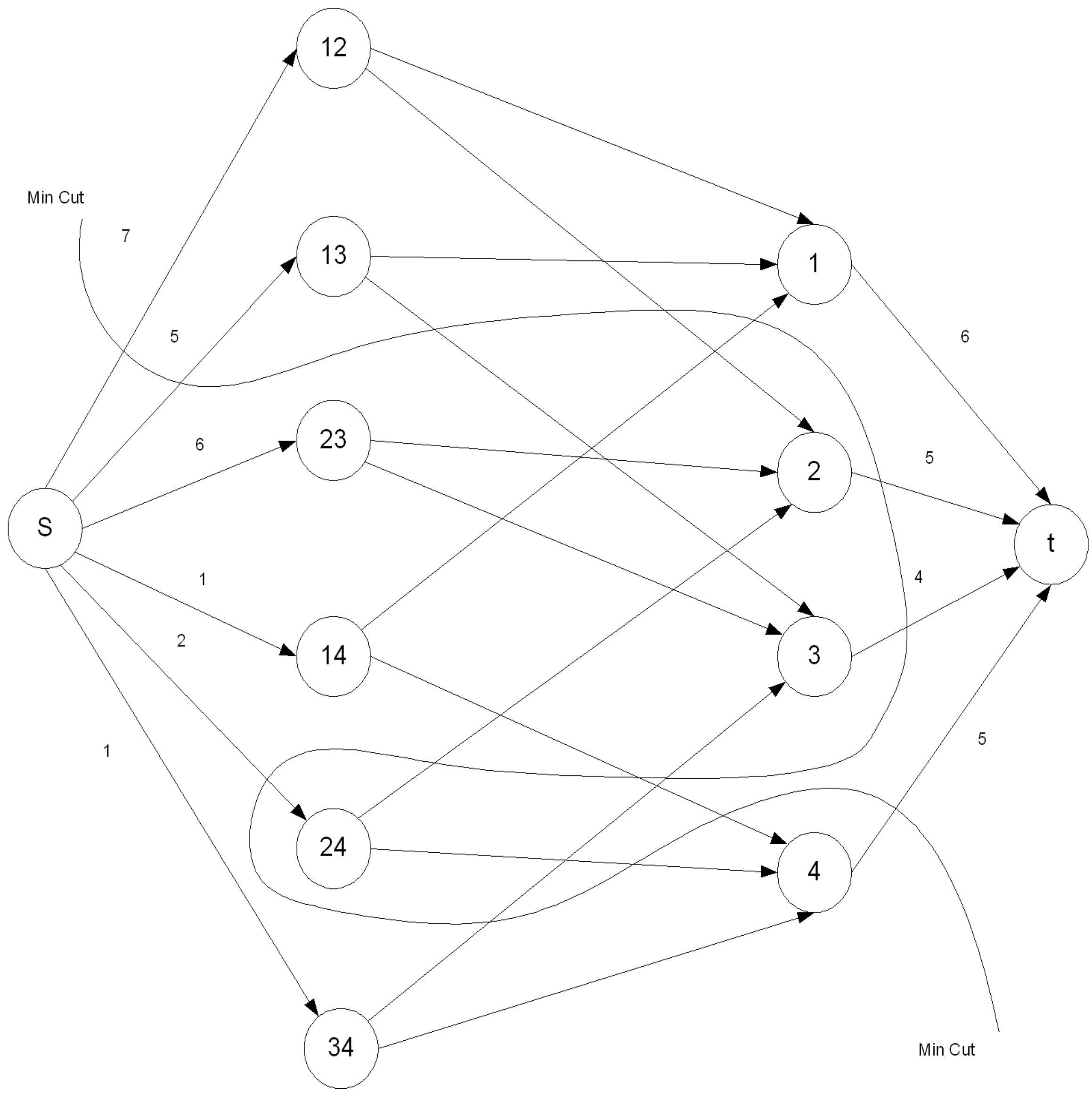

Figure 6.65: The site selection problem as a max flow problem.

2. Solve a problem in which one of these arcs is forced out of the tour. The objective function cannot decrease, so will have a new higher lower bound.

3. If the value of the new lower bound is a least as large as the value of any known feasible tour, we need not consider restricting any more arcs.

4. Repeat process of restrict ability arcs until we find a better feasible tour or prove that no further restrictions can be better.

6.10 Examples: TSP, Branch and Bound

These are examples of the salesman problem.

1. Computer wiring. A computer interface consists of several modules. On each module are located several pins. A given subset of pons has to be interconnected by wires. Because of the possible modifications and corrections and of the small size of the pin, at most two wires can be attached to any pin. In order to avoid signal cross talk and to improve the ease and neatness of wire ability, the total wire length must be minimized.

2. Circuit board drilling. Metalica is a Greek manufacturer of printer circuit board (PCB). Holes must be drilled in the PCB's at locations that correspond to pins where electronic components will later be soldered on the board. A typical PCB might have 500 pin placements. Most of the drilling is performed by programmable machines. Finding the optimal drilling sequence is a TSP. By solving the TSP problems for PCB's on a personal computer, Metalica reduced the time required to drill boards by 30%.

3. Order picking in a warehouse. Note: on the TSP problem, we can never travel through the same point twice.
   Let's use the optimum solution technique, branch and bound. Consider the example of an asymmetric matrix problem in the table below.

	1	2	3	4	5
1	—	3	7	6	2
2	4	—	11	9	6
3	3	6	—	1	5
4	5	5	3	—	4
5	6	2	7	6	—

   Answer: 1-3-4-5-2-1 with a distribution of 18. The greedy heuristic algorithm went through the following $(1,5),(5,2),(2,4),(4,3),(3,1) = 19$. $z^* \leq 19, z^*$ is optimal. The lower bound (but not optimal) is found by MST on a symmetric matrix.

The general idea of the branch and bound algorithm is:

1. Solve a relaxation of the TSP. If the solution is a feasible tour, stop. It must be optimal. If the solution is not a tour, then it is a lower bound. At least one of the arcs in this solution which causes the in-feasibility cannot be included in the optimal solution.

2. Solve a problem in which one of these arcs is forced out of the tour. The objective function cannot decrease, so will have a new higher lower bound.

3. If the value of the new lower bound is at least as large as the value of any known feasible tour, we need not consider restricting any more arcs.

4. Repeat the process of restrict ability arcs until we find a better feasible tour or prove that no further restrictions can be better.

Example: Solve the following assignment problem.

$$\min z = 3x_{12} + 7x_{13} + 6x_{14} + 2x_{15}$$

$$s.t. \sum x_{ij} = 1, \forall i$$

$$s.t. \sum x_{ij} = 1, \forall j$$

Solution: Consider the two sub-tours: 1-5-2-1, and 3-4-3, $z = 12$. At least one of these arc's will not be in the optimal tour. See Figure 6.66 for a branch and bound tree.

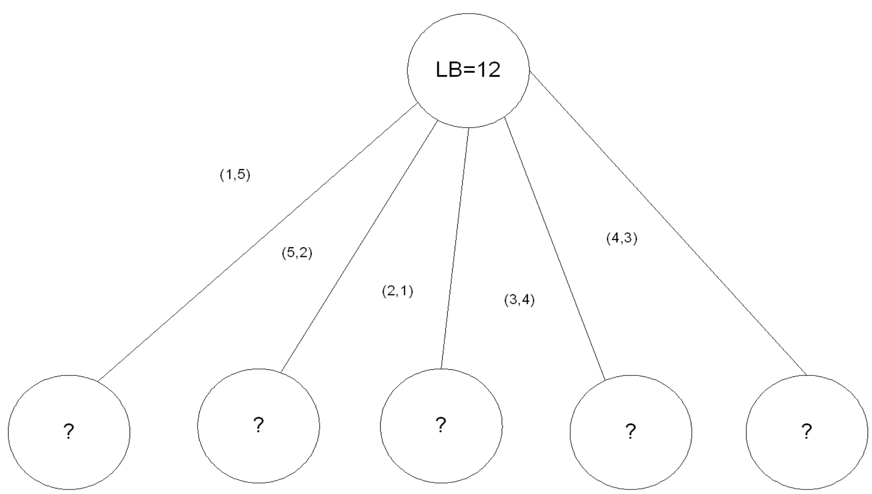

Figure 6.66: A branch and bound tree

Example: Setting the cost of $(1,5) = 99,999$ yields the path 2-3-4-5-2-1 with $z = 18$. This solution is feasible. Are we done? This solution is an upper bound. We now know $12 < z^* \leq 18$. We now exclude (5,2). Solution 1-2-5-1, 4-3-4, $z = 19$. This solution is infeasible and $z > 18$. So abandon arc (2,1). Result: 5-1-2-5, 4-3-4, $z = 19$. Same for exclude (3, 4). Now exclude (4,3) to get 1-3-4-5-2-1. This solution must be optimal (same as before $z = 18$.) If we had found a node with a lower bound smaller than the best known upper bound, we would have had to continue branching by excluding more arcs *until* we either had found a better tour or proved we cannot. Note that a good lower bound from a known feasible solution is very helpful.

6.11 Minimum Cost Network Flow Problem

Consider production scheduling as a minimum cost network flow problem (MCNFP). Polyester fiber is used in manufacturing a textile fabric. An initial inventory of 10 unites is on hand. The maximum inventory capacity is 20 units. An inventory of 8 units is required at the end of the next 4 month planning period. The current price of the fiber is \$6.00 per unit, but its is expected to increase by 1 each month. The unit cost of keeping an inventory in stock is \$0.25 per unit per month. Demands are 12, 19, 15, 20 in the next 4 months. Production varies from 14 to 18 units each month. Let the network arc parameters be (L_{ij}, U_{ij}, c_{ij}). This is drawn as an MCNFP in Figure 6.67.

Example: Consider the traveling salesman problem in Figure 6.68. The driving time (in minutes) between locations is

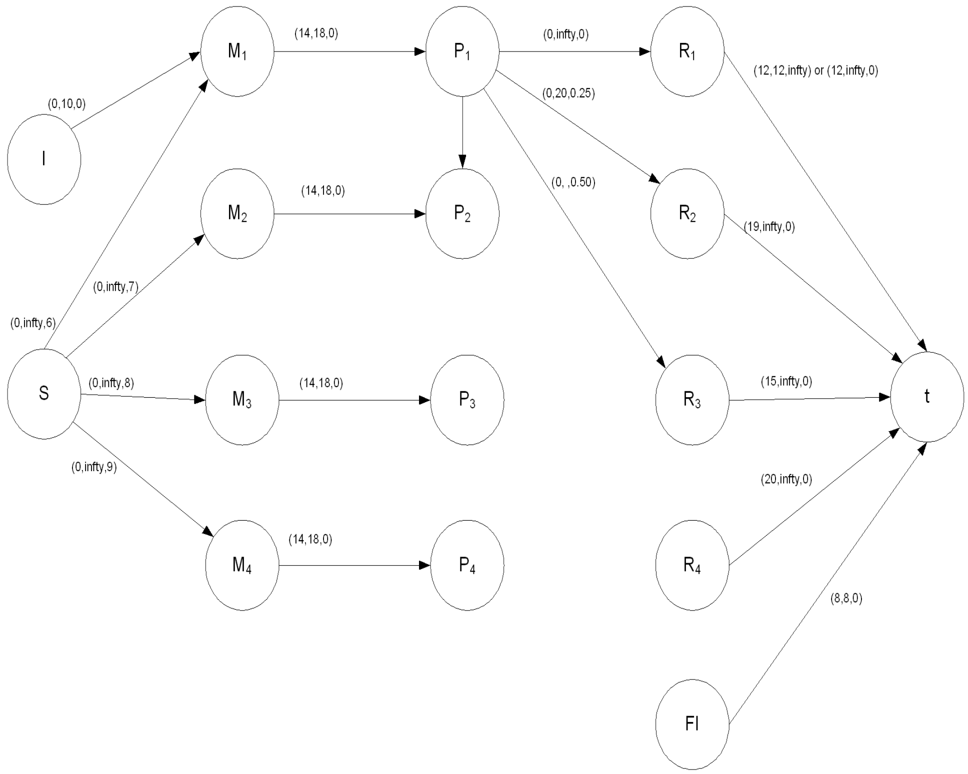

Figure 6.67: Production scheduling as an MCNFP problem.

	1	2	3	4	5	6	7
1	–	35	20	25	40	30	35
2	35	–	15	50	45	65	70
3	20	15	–	25	45	50	55
4	25	50	25	–	65	45	40
5	40	45	45	65	–	35	45
6	30	65	50	45	35	–	10
7	35	70	55	40	45	10	–

where the columns are interpreted as 'driving to' and the rows are interpreted as 'driving from.' Using the nearest neighbor technique, scan the table; find two locations closest to each other, and connect them. Cross out the columns and rows based on this idea until you have a feasible solution. Choose $T(7,6)$. Therefore, the van drives from 7 to 6. Cross out row 7 and column 6 and element $(6,7)$. Choose $T(2,3)$. Then $T(3,1), 3 \to 2 \to 1$, and $7 \to 6, 6 \to 5$. The final solution to the problem is $1 \to 4 \to 7 \to 6 \to 5 \to 2 \to 3 \to 1$, and the total length is 190. With this approach, continually look for cycles. See Figure 6.69.

Now try the nearest neighbor technique on our other example (non-symmetric).

	1	2	3	4	5
1	–	3	7	6	2
2	4	–	1	9	6
3	2	6	–	1	5
4	5	5	3	–	4
5	6	2	7	6	–

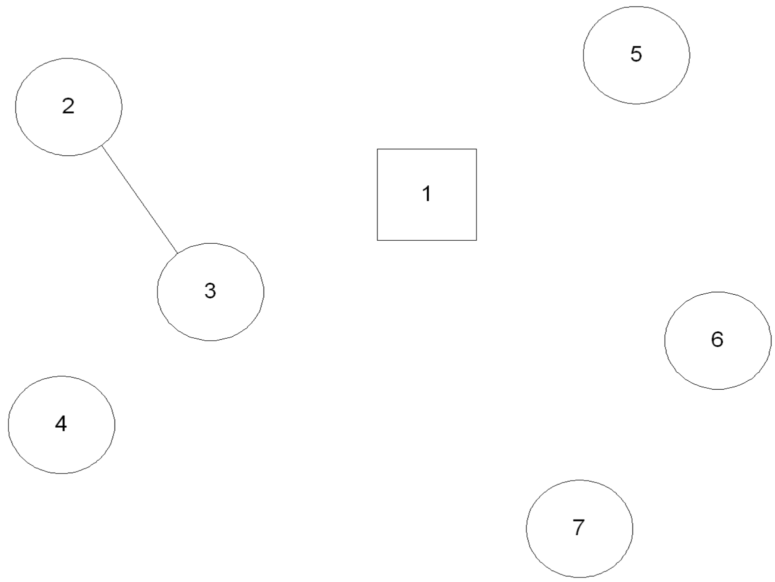

Figure 6.68: Traveling salesman problem as an MCNFP.

A variation of this technique is after choosing (i, j) only look at the j-th row; choose (j, k). No sub-cycle problem. $(3, 4), (4, 5), (5, 2), (2, 1), (1, 3)$. $1+4+2+4+7 = 18$ is the optimal solution, but is not guaranteed.

Another possible heuristic technique is called the cheapest insertion heuristic. Consider the graph in Figure 6.70.

$k = c_{ik} + c_{jk} - c_{ij}$ is the net cost of eliminating (i, j) and adding (k, j) to the cycle. Begin at any city; choose its nearest neighbor. Create a sub-tour joining *here* two cities. Replace an arc in the sub-tour by the combination of two arcs (i, j). (i, j) becomes (i, k) and (k, j) where k is chosen to increase the cost by the smallest amount. At each step the net increase is $c_{ik} + c_{kj} - c_{ij}$. Continue until a tour is found. This heuristic involves much more work that the nearest neighbor heuristic.

6.12 Homework and Answers

The names Joan, Jen Mauger and Paige Burger appear as group members in my notes. I don't remember Joan's last name, as I am typesetting these notes in 2006 (memory failure).

Since this problem set covers a month of material, it is worth 150 points, not 100. The last two problem sets will be worth only 75 points each or else we will combine them into another 150 point problem set, for a total of four. Ground rules are the same. Be sure to explain your assumptions and your answers.

1. (a) Find a lower bound (infeasible) solution using the assignment problem Hungarian algorithm and a feasible upper bound using the nearest neighbor heuristic, for the traveling salesman problem.

   Solution: The problem given was to find an infeasible lower bound and a feasible upper bound to a matrix of distances. The infeasible lower bound was determined using the Hungarian algorithm, and the feasible upper bound was determined with the nearest neighbor heuristic. The distance matrix is as follow:

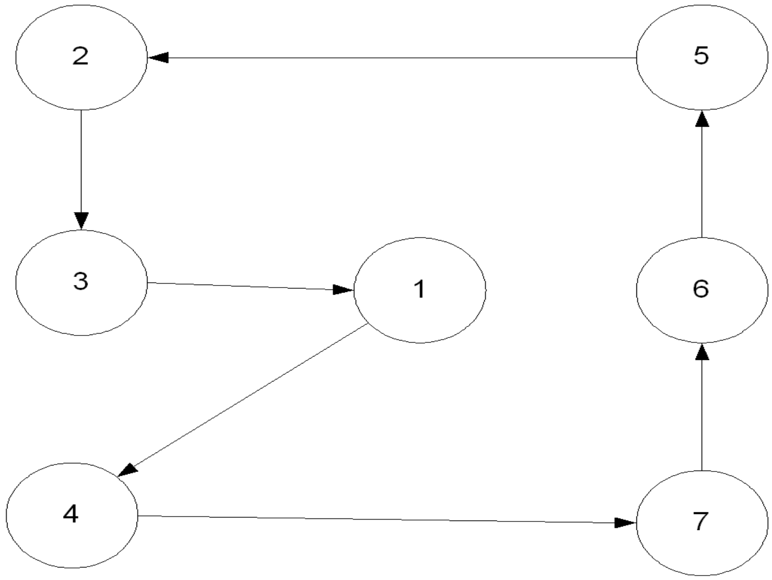

Figure 6.69: The traveling salesman solution.

	1	2	3	4	5	6
1	—	27	43	16	30	26
2	7	—	16	1	30	25
3	20	13	—	35	6	0
4	21	16	25	—	18	18
5	12	46	27	48	—	5
6	23	5	5	9	5	—

The feasible upper bound is 70 which has the following tour: $(3, 6)$, $(2, 4)$, $(6, 5)$, $(5, 1)$, $(1, 2)$, $(4, 3)$, $0+\ 1+\ 5+\ 12 + 27 + 25 = 70$. The infeasible lower bound is as follow:

$$c = \begin{bmatrix} - & 27 & 43 & 16 & 30 & 26 \\ 7 & - & 16 & 1 & 30 & 25 \\ 20 & 13 & - & 35 & 5 & 0 \\ 21 & 16 & 25 & - & 18 & 18 \\ 12 & 46 & 27 & 48 & - & 5 \\ 23 & 5 & 5 & 9 & 5 & - \end{bmatrix}$$

$16, 1, 5, 16, 5, 5.$

$$\begin{bmatrix} - & 11 & 27 & 0 & 14 & 10 \\ 6 & - & 15 & 0 & 29 & 24 \\ 15 & 8 & - & 30 & 0 & 0 \\ 5 & 0 & 9 & - & 2 & 2 \\ 7 & 41 & 22 & 43 & - & 0 \\ 18 & 0 & 0 & 4 & 0 & - \end{bmatrix}$$

Consider rows 1, 2, 4, 5. Consider column 3. No complete assignment done. Rows of zeroes: 1, 1, 2, 1, 1, 3. Column of zeroes: 0, 2, 1, 2, 2, 2. The minimum uncovered value is 2.

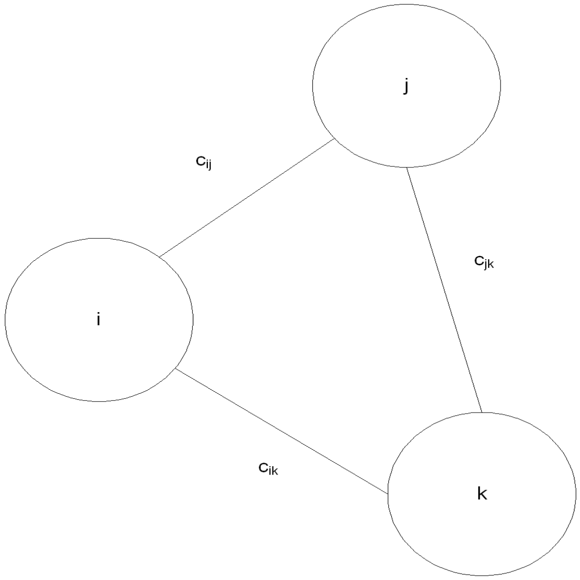

Figure 6.70: Cheapest insertion heuristic.

$$\begin{bmatrix} - & 9 & 25 & 0 & 12 & 8 \\ 4 & - & 13 & 0 & 27 & 22 \\ 13 & 10 & - & 32 & 0 & 0 \\ 3 & 0 & 7 & - & 0 & 0 \\ 5 & 39 & 20 & 41 & - & 0 \\ 16 & 0 & 0 & 6 & 0 & - \end{bmatrix}$$

Consider rows 1, 2, 4. Consider column 3. Rows of zeroes: 1, 1, 2, 3, 1, 3. Column of zeroes: 0, 2, 1, 2, 3, 3. The smallest uncovered number is 4. So,

$$\begin{bmatrix} - & 5 & 21 & 0 & 8 & 4 \\ 0 & - & 9 & 0 & 23 & 18 \\ 11 & 6 & - & 28 & 0 & 0 \\ -1 & 0 & 3 & - & 0 & 0 \\ 1 & 35 & 16 & 37 & - & 0 \\ 12 & 0 & 0 & 10 & 0 & - \end{bmatrix}$$

So, the path $(1,4),(4,2),(2,1),(3,5),(5,6),(6,3)$ has a lower bound of 54.

(b) Write the linear program for this traveling salesman problem — you can omit some of the constraints once the pattern is clear.

Solution: We were asked to write an LP for the problem. Minimize

$$7x_{21} + 20x_{31} + 21x_{41} + 12x_{51} + 23x_{61} + 27x_{12} + 13x_{32} + 16x_{42} + 46x_{52} + 5x_{62} + \cdots +$$

$$26x_{16} + 25x_{26} + 18x_{46} + 5x_6$$

Subject to the following constraints:

$$\begin{aligned}
&x_{21} + x_{31} + x_{41} + x_{51} + x_{61} &&= 1 \\
&x_{12} + x_{32} + x_{42} + x_{52} + x_{62} &&= 1 \\
&\vdots && \vdots \\
&x_{16} + x_{26} + x_{36} + x_{46} + x_{56} &&= 1 \\
&x_{12} + x_{13} + x_{14} + x_{15} + x_{16} &&= 1 \\
&x_{21} + x_{23} + x_{24} + x_{25} + x_{26} &&= 1 \\
&\vdots && \vdots \\
&x_{61} + x_{62} + x_{63} + x_{64} + x_{65} &&= 1
\end{aligned}$$

$x = \{1, 2, 3, 4, 5, 6\}$.

$$\begin{aligned}
&S = \{1\}, \{2\}, \{3\}, \{4\}, \{5\}, \{6\}, \\
&\{1, 2\}, \{1, 3\}, \{1, 4\}, \cdots \{1, 6\}, \\
&\{2, 1\}, \{2, 3\}, \{2, 4\}, \cdots \{2, 6\}, \\
&\vdots \\
&\{6, 1\}, \{6, 2\}, \{6, 3\}, \cdots \{6, 5\}, \\
&\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \\
&\vdots \\
&\{1, 2, 3, 4, 5, 6\}.
\end{aligned}$$

Let $S = \{1\}$. Then, $X - S = \{2, 3, 4, 5, 6\}$.

$$x_{12} + x_{13} + x_{14} + x_{15} + x_{16} \geq 1.$$

Let $S = \{1, 2\} \Rightarrow X - S = \{3, 4, 5, 6\}$.

$$x_{13} + x_{14} + x_{15} + x_{16} + x_{23} + x_{24} + x_{25} + x_{26} \geq 1.$$

2. In the turn penalty algorithm, why is it not possible to add the penalty to each arc parameter and then solve by the shortest route algorithm? Create a simple turn — penalty problem and illustrate that this approach will not work.

   Solution: We were asked to explain why in the turn signal problem we cannot add the penalty to each arc parameter and then solve by the shortest route algorithm. We cannot apply that technique because an ambiguous network would be the result. Two values may be needed to be applied to some arc's in the network. One value corresponds to traversing the arc without a turn and the other value corresponds to traversing the arc with a turn. Below, is the value of arc $(4, 5) = 1 + 3$ (assume penalty of $3) + 2 = 6$ or $3 + 2 = 5$. See Figure 6.71. There are two ways to get to (4,5). That is 1-3-4 and 1-2-4.

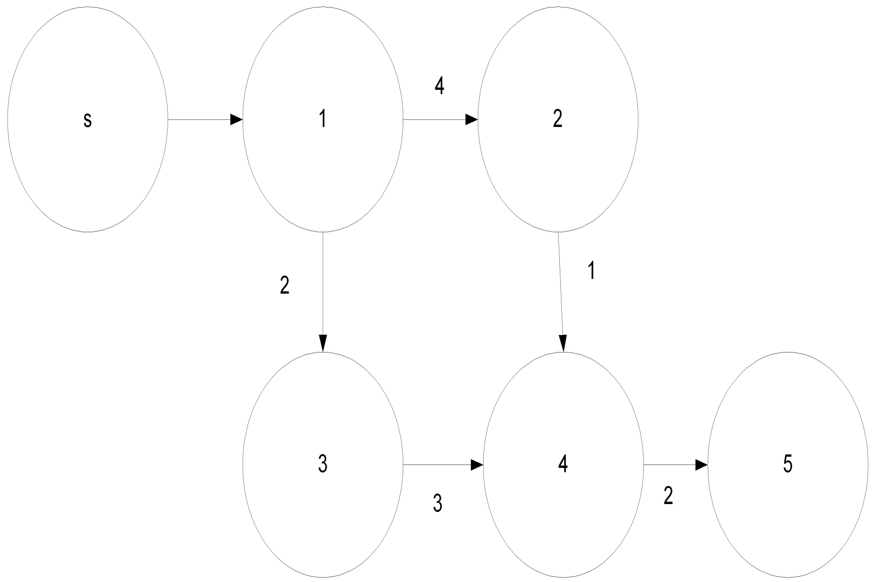

Figure 6.71: *This figure shows the turn signal problem.*

3. Problem 50, page 193 of the text book. For part (a), a feasible upper bound solution will do, but find the best one you can.

   Rail-Riders is interested in designing a high speed people mover system connecting six airline terminals in Space City. Regulations require that the high speed tracks not cross one another, in other words, Space City needs a closed circuit matrix below representing the distances in feet between terminal points. Rail-Riders would like to design a system that will incur the minimal cost while adhering to the regulation. Cost per foot is a constant $100. Consequently, to minimize the costs, we need to minimize the total distance of the path.

	1	2	3	4	5	6
1	–	870	910	796	860	712
2	870	–	1100	560	430	630
3	900	1100	–	270	600	–
4	796	560	270	–	300	850
5	850	430	600	300	–	370
6	712	630	250	850	370	–

   A feasible upper bound will suffice for Rail-Riders, but we should try to find the best upper bound.

   Using the nearest neighbor technique, I [Jen] shall find an upper bound using all six points as the starting terminal then choose the best of the six as our answer. The numbers will be expressed in the following diagram format.

```
path: A ---> # ---> # ---> # ---> # ---> # ---> # A (A = start/end)
feet:    """ +  """ +  """ +  """ +  """ +  """     = total distance
cost:                          (total distance)($100)  = total cost

path: 1 ---> 6 --> 3 --> 4 --> 5 --> 2 --> 1      (1 = start/end)
```

```
feet:    712 + 250 + 270 + 300 + 430 + 870          = 2832 ft.
cost:                                (2832)($100)  = $283,200

path: 2 ---> 5 --> 4 --> 3 --> 1 --> 6 --> 2       (2 = start/end)
feet:    430 + 300 + 270 + 900 + 712 + 630          = 3242 ft.
cost:                                (3242)($100)  = $324,000

path: 3 ---> 4 --> 5 --> 6 --> 2 --> 1 --> 3       ( = start/end)
feet:    270 + 300 + 370 + 630 + 870 + 910          = 3350 ft.
cost:                                (3350)($100)  = $335,000

path: 4 ---> 3 --> 5 --> 6 --> 2 --> 1 --> 4       (4 = start/end)
feet:    270 + 600 + 370 + 630 + 870 + 796          = 3536 ft.
cost:                                (3536)($100)  = $353,600

path: 5 ---> 4 --> 3 --> 1 --> 6 --> 2 --> 5       (5 = start/end)
feet:    300 + 270 + 900 + 712 + 630 + 430          = 3242 ft.
cost:                                (3242)($100)  = $324,200

path: 6 ---> 3 --> 4 --> 5 --> 2 --> 1 --> 6       (6 = start/end)
feet:    250 + 270 + 300 + 430 + 870 + 712          = 2832 ft.
cost:                                (2832)($100)  = $283,200
```

Note that the cycles starting with terminals 1 and 6 yielded the same upper bound, as did the cycles starting with 2 and 5. The former set clearly gives the best upper bound of 2832 feet, or a $283,200 cost.

The regulation in the question stated that the people mover tracks could not cross. Although the question is trying to imply they wish a traveling salesman problem answer, the regulation wording does not seem to represent this. The regulation cannot be completely fulfilled without a picture, or network, of the postions of the terminals. For example, if the terminals are arranged as shown in Figure 6.72, our upper bound would not be feasible as the tracks cross. But, if the terminals were arranged as shown in Figure 6.73, the upper bound will satisfy the regulation. The solving process above assumed that the terminals were floating and could be made permanent after the solution was achieved. More likely however, the terminals are already placed prior to solving a people mover dilemma. Consequently, there are only two possible paths, one of which must be optimal given the positioning of the nodes. We no longer have a typical traveling salesman problem due to the regulation constraint. Supposing the treminals are laid out according to the network in Figure 6.72, the optimal path must be one of the following. Note that any terminal can be chosen as the starting point and the same two paths will result.

```
path: 1 ---> 2 --> 3 --> 4 --> 5 --> 6 --> 1       (1 = start/end)
feet:    870 + 1100 + 270 + 300 + 370 + 712          = 3622 ft.
cost:                                (3622)($100)  = $362,200

path: 1 ---> 6 --> 5 --> 4 --> 3 --> 2 --> 1       (1 = start/end)
feet:    712 + 370 + 300 + 270 + 1100 + 870          = 3622 ft.
cost:                                (3622)($100)  = $362,200
```

In this case, the distance of the paths ended up being identical. But we cannot assume this to be the ase given any combination of placement of the terminals since the distance matrix is not completely symmetric.

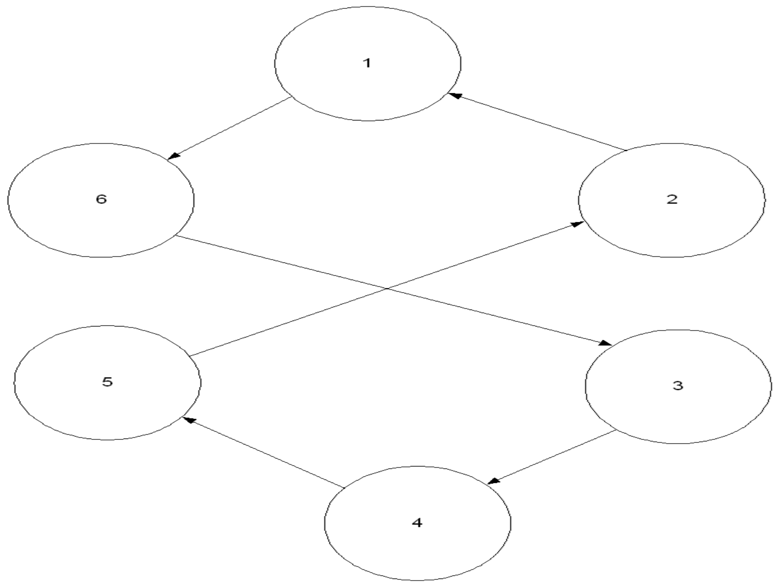

Figure 6.72: *This figure shows one possible arrangement of terminal nodes.*

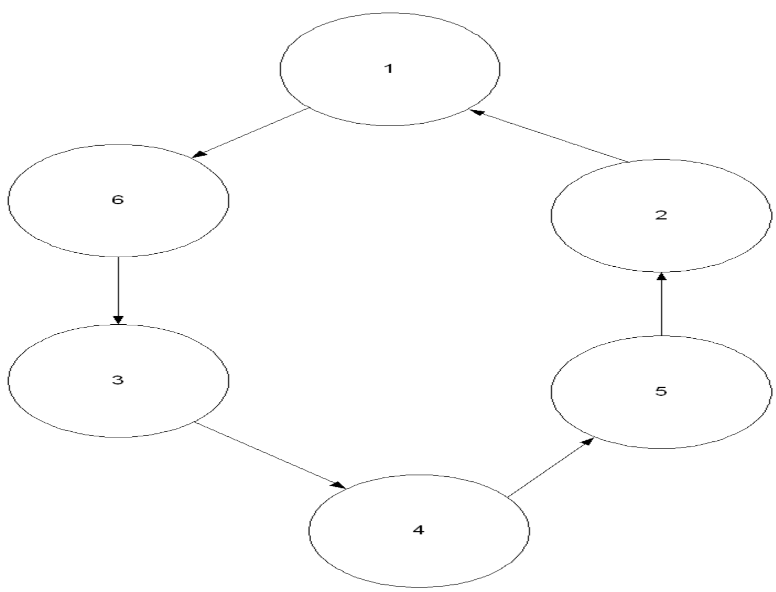

Figure 6.73: *This figure shows a second possible arrangement of terminal nodes.*

Solution to part (b). Rail-Riders wishes to propose an alternate design. If a hub node is introduced and placed in a central position, the people mover can be designed as a hub-and-spoke system with each terminal having only one path entering it which comes from the hub and only one path leaving it which goes to the hub. The distance between each terminal and the hub is summarized in the following table.

Terminal	1	2	3	4	5	6
Hub	150	175	210	180	175	190

Design the new system at minimal cost and compare the results to those in Part (a). The network shown in Figure 6.74 depicts the bicycle spoke type diagram. In this case, there is no minimum path to decide upon because according to the companies description, the only possible path is that in Figure 6.74. Unless of course, the company wishes to consider adding pathways between the nodes that do not go through the hub. But this would not yield a minimum cost. Since there will be two paths, one in each direction, we must add twice the distances in the table to obtain the minimum distance: $2(150+175+210+180+175+190) = 2160$. So, the cost would be $(100)(2160) = \$216,000$. This cost is considerably less than that in Part (a). Additionally, the hub and spoke design is more efficient in terms of time it takes to get from one node to another. Using the first best upper bound path from Part (a): $1 -- > 6 -- > 3 -- > 4 -- > 5 -- > 2 -- > 1$. If a person were at terminal 6, (s)he would have to go through all of the terminals, a distance of 2832 feet, in order to reach terminal 1. But, in the second design, the person would simply go from 6 to the hub, and then from the hub to 1 at a distance of 340 feet. Thus, for several reasons, the alternate design is clearly more efficient and less costly. Rail Riders should build the second system over the first.

4. Problem 52, page 194 of the text book. Use the Hungarian algorithm.

   Solution: In this problem, we were asked to find the minimal cost schedule of assigning jobs to machines. Four job orders have been received in the shop. Five machines are available. The cost to make the job at different machines is given in the following matrix.

	1	2	3	4	5
1	12	14	12	18	0
2	16	10	10	16	0
3	10	8	8	14	0
4	8	12	16	12	0
5	14	10	18	14	0

   The solution using the Hungarian algorithm results in the following assignments.

Machine	Job
1	5
2	2
3	3
4	1
5	4

   This has a cost of $10 + 8 + 8 + 14 = 40$. Also consider an alternate assignment of

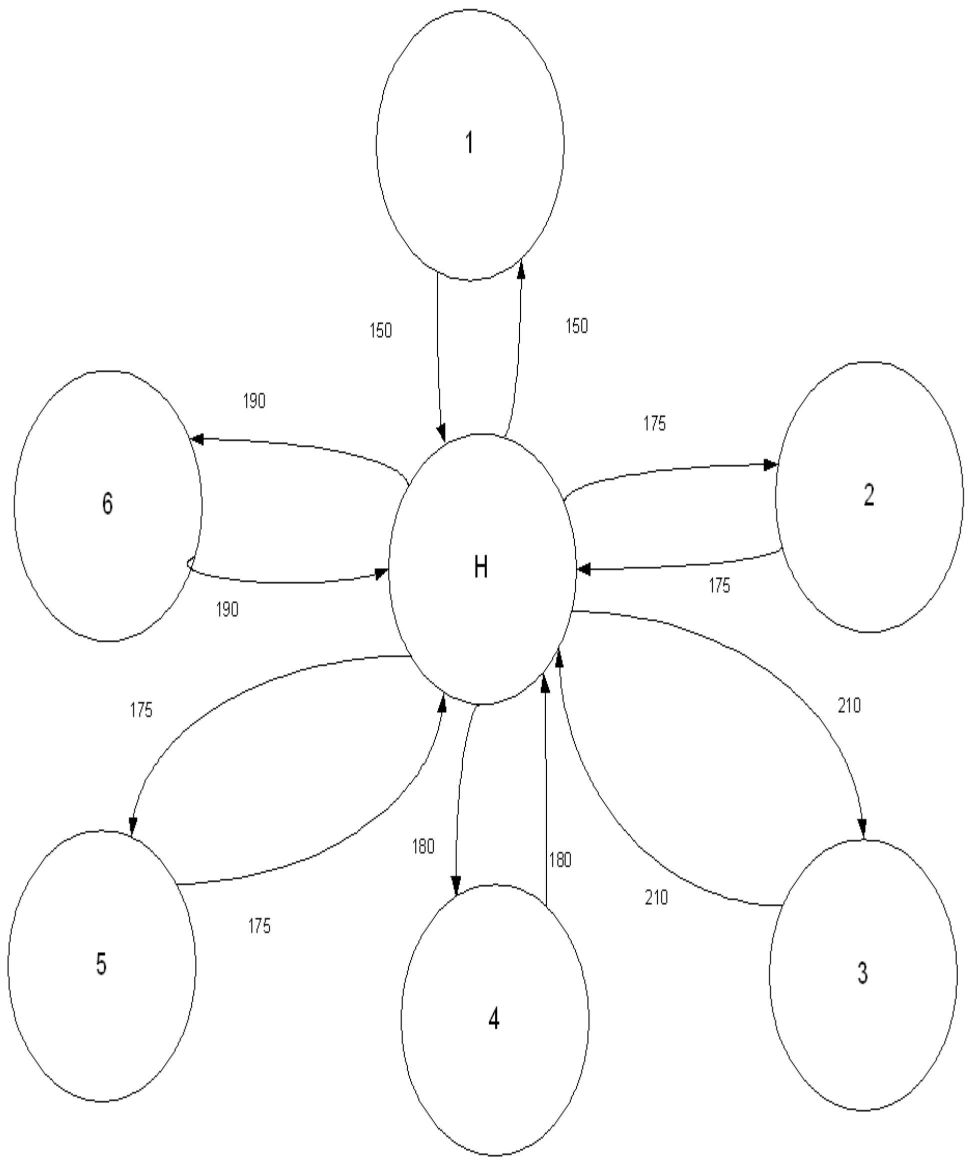

Figure 6.74: *This figure shows the optimal configuration for Rail Riders.*

Machine	Job
4	1
3	2
2	3
5	4

which has a cost of $8 + 8 + 10 + 14 = 40$.

Solution:

$$c = \begin{bmatrix} 12 & 14 & 12 & 18 & 0 \\ 16 & 10 & 10 & 16 & 0 \\ 10 & 8 & 8 & 14 & 0 \\ 8 & 12 & 16 & 12 & 0 \\ 14 & 10 & 18 & 14 & 0 \end{bmatrix}$$

The minimum values in the columns are 8, 8, 8, 12, 0.

$$\begin{bmatrix} 4 & 6 & 4 & 6 & 0 \\ 8 & 2 & 2 & 4 & 0 \\ 2 & 0 & 0 & 2 & 0 \\ 0 & 4 & 8 & 0 & 0 \\ 6 & 2 & 10 & 2 & 0 \end{bmatrix}$$

Consider rows 1, 2, 5. Consider columns 1, 2, 3, 4. No assignment is made to cells $(3, 3)$ and $(4, 4)$. Row zeroes: 1, 1, 3, 3, 1. Column zeroes: 1, 1, 1, 1, 5. Choose column 5. Therefore the minimum cost showing is 2.

$$\begin{bmatrix} 2 & 4 & 2 & 4 & 0 \\ 6 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 2 \\ 0 & 2 & 6 & 0 & 2 \\ 4 & 0 & 8 & 0 & 0 \end{bmatrix}$$

Row 1 has one un crossed zero. $(1, 5), (2, 2), (3, 3), (4, 1), (5, 4)$.

5. Problem 22, parts (a) and (b) only in the text book. Problem 23, page 185.

   Solution: In the network in Figure 6.75, find:

   (a) The max flow from 2 to 10. Solution: Figure 6.76 shows the network and work for finding the maximum flow from node 2 to 10. The arcs labels represent "(remaining capacity, amount sent)." The paths chosen and their respective flow amounts are below; the maximum flow is $16 + 19 + 6 + 10 = 51$.

   So, the maximum capacity chain from nodes 2 to 10 path is $2 \rightarrow 5 \rightarrow 7 \rightarrow 8 \rightarrow 10$ with a capacity of 19.

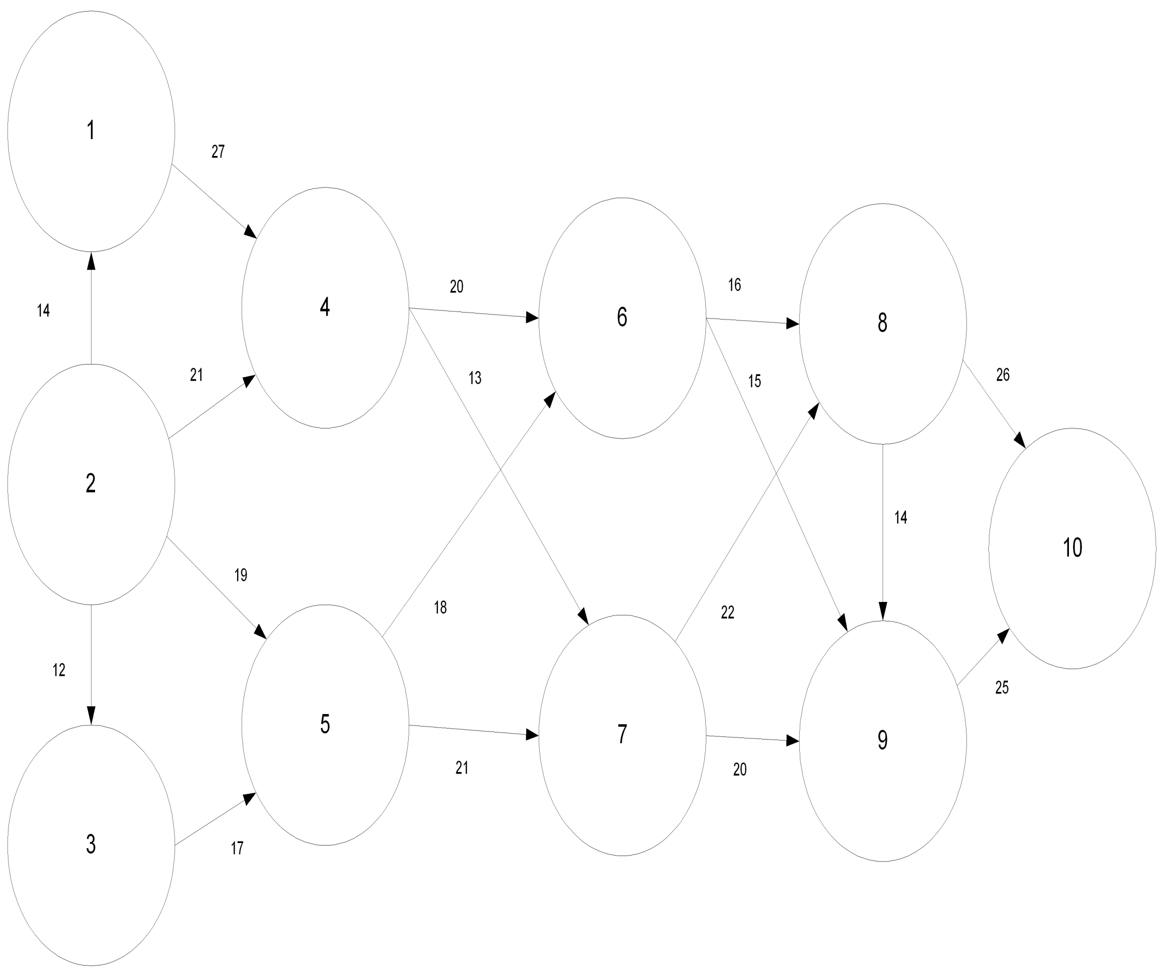

Figure 6.75: *This figure shows the network problem to be solved.*

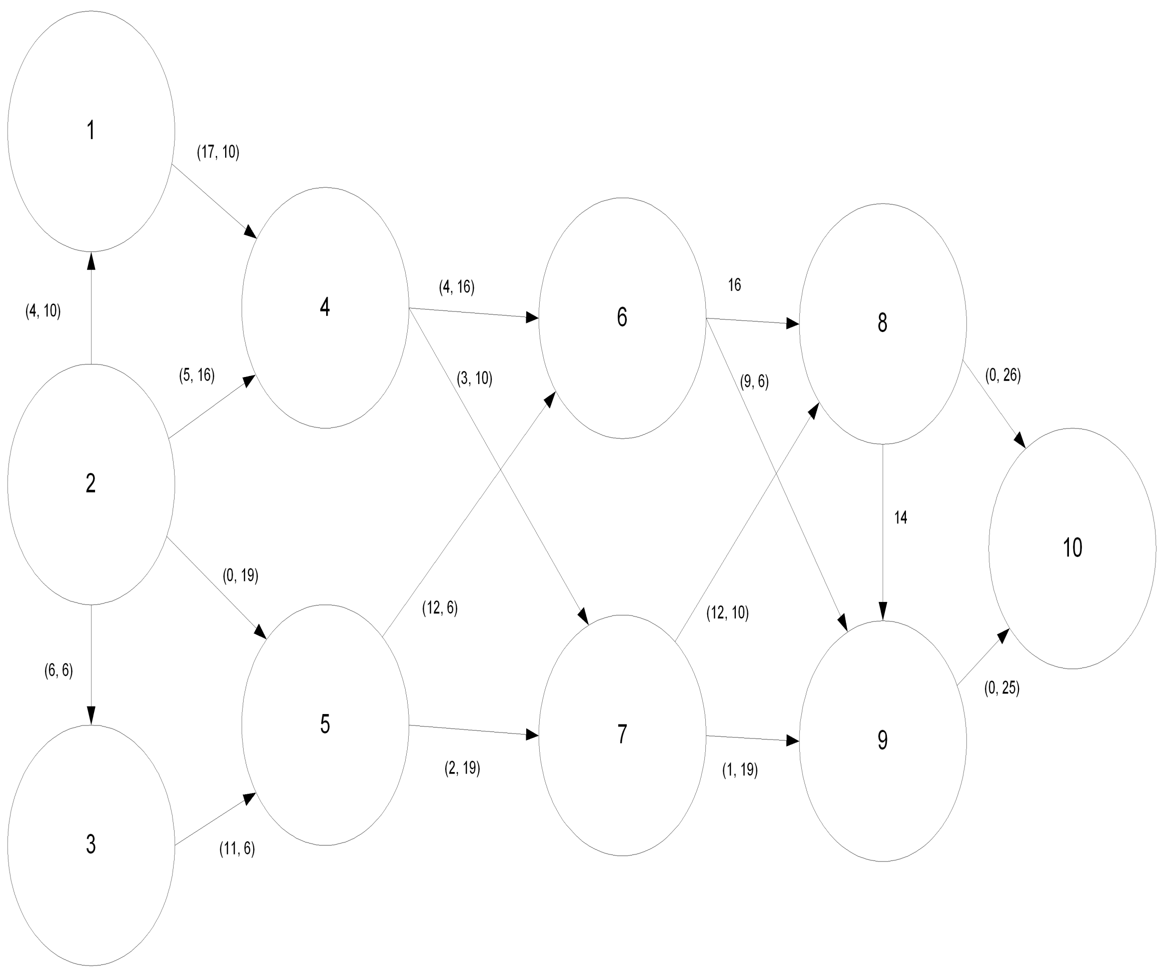

Figure 6.76: *This figure shows an iteration of the network problem being solved.*

```
path1: 2 --> 4 --> 6 --> 8 --> 10          yield = 16
path2: 2 --> 5 --> 7 --> 9 --> 10          yield = 19
path3: 2 --> 3 --> 5 --> 6 --> 9 --> 10    yield =  6
path4: 2 --> 1 --> 4 --> 7 --> 8 --> 10    yield =  10
```

(b) The max-capacity from 2 to 10. Solution: Find the maximal capacity chain from 2 to 10. I [Jen] found out that we did not have to use the text algorithm after I [Jen] had already solved the problem and written up the following text and diagrams. So, I [Jen] left it in!

The next few tables show the capacity and route matrices used for the 10 iterations of the maximal capacity chain algorithm. The initial matrices are shown on the first table. These matrices remain the same through the first 3 iterations. For the matrices for iterations 4-9, on the following tables, the following code holds: if the capacity matrix has a blank entry, the value is assumed to be negative infinity, if the route matrix has a blank entry, it is assumed to carry the same numbers as in the first route matrix — i.e. I only entered numbers where changes occurred during the iterations. On the final table, the final matrices, which also correspond to iteration 10, are written in full. Reading the entry in the 2-nd row, 10-th column, we see the maximum capacity chain from node 2 to node 10 will have a length of 19. The path can be easily traced using the route matrix. The notation r_{ij} means the i-th row, j-th column entry.

```
r2,10 =  8  2 --> 10 via 8
r8,10 = 10  8 --> 10 direct
r2,8  =  7  2 --> 8 via 7
r7,8  =  8  7 --> 8 direct
r2,7  =  5  2 --> 7 via 5
r5,7  =  7  5 --> 7 direct
r2,5  =  5  2 --> 5 direct
```

This is the initial capacity matrix.

$$
\left[\begin{array}{c|cccccccccc}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
\hline
1 & 0 & -\infty & -\infty & 27 & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty \\
2 & 14 & 0 & 12 & 21 & 19 & -\infty & -\infty & -\infty & -\infty & -\infty \\
3 & -\infty & -\infty & 0 & -\infty & 17 & -\infty & -\infty & -\infty & -\infty & -\infty \\
4 & -\infty & -\infty & -\infty & 0 & -\infty & 20 & 13 & -\infty & -\infty & -\infty \\
5 & -\infty & -\infty & -\infty & -\infty & 0 & 18 & 21 & -\infty & -\infty & -\infty \\
6 & -\infty & -\infty & -\infty & -\infty & -\infty & 0 & -\infty & 16 & 15 & -\infty \\
7 & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & 0 & 22 & 20 & -\infty \\
8 & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & 0 & 14 & 26 \\
9 & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & 0 & 25 \\
10 & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & 0
\end{array}\right]
$$

This is the initial route matrix.

	1	2	3	4	5	6	7	8	9	10
1	1	2	3	4	5	6	7	8	9	10
2	1	2	3	4	5	6	7	8	9	10
3	1	2	3	4	5	6	7	8	9	10
4	1	2	3	4	5	6	7	8	9	10
5	1	2	3	4	5	6	7	8	9	10
6	1	2	3	4	5	6	7	8	9	10
7	1	2	3	4	5	6	7	8	9	10
8	1	2	3	4	5	6	7	8	9	10
9	1	2	3	4	5	6	7	8	9	10
10	1	2	3	4	5	6	7	8	9	10

The initial capacity and route matrices remain the same as the initial ones for iterations 1, 2, and 3 or $j = 1, 2, 3$.

Iteration 4 $(j = 4)$:

	1	2	3	4	5	6	7	8	9	10
1	0	$-\infty$	$-\infty$	27	$-\infty$	20	13	$-\infty$	$-\infty$	$-\infty$
2	14	0	12	21	19	20	13	$-\infty$	$-\infty$	$-\infty$
3	$-\infty$	$-\infty$	0	$-\infty$	17	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$
4	$-\infty$	$-\infty$	$-\infty$	0	$-\infty$	20	13	$-\infty$	$-\infty$	$-\infty$
5	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	18	21	$-\infty$	$-\infty$	$-\infty$
6	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	$-\infty$	16	15	$-\infty$
7	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	22	20	$-\infty$
8	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	14	26
9	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	25
10	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0

	1	2	3	4	5	6	7	8	9	10
1	1	2	3	4	5	4	4	8	9	10
2	1	2	3	4	5	4	4	8	9	10
3	1	2	3	4	5	6	7	8	9	10
4	1	2	3	4	5	6	7	8	9	10
5	1	2	3	4	5	6	7	8	9	10
6	1	2	3	4	5	6	7	8	9	10
7	1	2	3	4	5	6	7	8	9	10
8	1	2	3	4	5	6	7	8	9	10
9	1	2	3	4	5	6	7	8	9	10
10	1	2	3	4	5	6	7	8	9	10

Iteration 5 $(j = 5)$:

	1	2	3	4	5	6	7	8	9	10
1	0	$-\infty$	$-\infty$	27	$-\infty$	20	13	$-\infty$	$-\infty$	$-\infty$
2	14	0	12	21	19	20	19	$-\infty$	$-\infty$	$-\infty$
3	$-\infty$	$-\infty$	0	$-\infty$	17	17	17	$-\infty$	$-\infty$	$-\infty$
4	$-\infty$	$-\infty$	$-\infty$	0	$-\infty$	20	13	$-\infty$	$-\infty$	$-\infty$
5	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	18	21	$-\infty$	$-\infty$	$-\infty$
6	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	$-\infty$	16	15	$-\infty$
7	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	22	20	$-\infty$
8	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	14	26
9	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	25
10	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0

	1	2	3	4	5	6	7	8	9	10
1	1	2	3	4	5	4	4	8	9	10
2	1	2	3	4	5	4	5	8	9	10
3	1	2	3	4	5	5	5	8	9	10
4	1	2	3	4	5	6	7	8	9	10
5	1	2	3	4	5	6	7	8	9	10
6	1	2	3	4	5	6	7	8	9	10
7	1	2	3	4	5	6	7	8	9	10
8	1	2	3	4	5	6	7	8	9	10
9	1	2	3	4	5	6	7	8	9	10
10	1	2	3	4	5	6	7	8	9	10

Iteration 6 ($j = 6$) :

	1	2	3	4	5	6	7	8	9	10
1	0	$-\infty$	$-\infty$	27	$-\infty$	20	13	16	15	$-\infty$
2	14	0	12	21	19	20	19	16	15	$-\infty$
3	$-\infty$	$-\infty$	0	$-\infty$	17	17	17	16	15	$-\infty$
4	$-\infty$	$-\infty$	$-\infty$	0	$-\infty$	20	13	16	15	$-\infty$
5	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	18	21	16	15	$-\infty$
6	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	$-\infty$	16	15	$-\infty$
7	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	22	20	$-\infty$
8	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	14	26
9	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	25
10	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0

	1	2	3	4	5	6	7	8	9	10
1	1	2	3	4	5	4	4	6	6	10
2	1	2	3	4	5	4	5	6	6	10
3	1	2	3	4	5	5	5	6	6	10
4	1	2	3	4	5	6	7	6	6	10
5	1	2	3	4	5	6	7	6	6	10
6	1	2	3	4	5	6	7	8	9	10
7	1	2	3	4	5	6	7	8	9	10
8	1	2	3	4	5	6	7	8	9	10
9	1	2	3	4	5	6	7	8	9	10
10	1	2	3	4	5	6	7	8	9	10

Iteration 7 ($j = 7$) :

	1	2	3	4	5	6	7	8	9	10
1	0	$-\infty$	$-\infty$	27	$-\infty$	20	13	16	15	$-\infty$
2	14	0	12	21	19	20	19	19	19	$-\infty$
3	$-\infty$	$-\infty$	0	$-\infty$	17	17	17	17	17	$-\infty$
4	$-\infty$	$-\infty$	$-\infty$	0	$-\infty$	20	13	16	15	$-\infty$
5	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	18	21	21	20	$-\infty$
6	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	$-\infty$	16	15	$-\infty$
7	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	22	20	$-\infty$
8	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	14	26
9	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	25
10	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0

	1	2	3	4	5	6	7	8	9	10
1	1	2	3	4	5	4	4	6	6	10
2	1	2	3	4	5	4	5	7	7	10
3	1	2	3	4	5	5	5	7	7	10
4	1	2	3	4	5	6	7	6	6	10
5	1	2	3	4	5	6	7	7	7	10
6	1	2	3	4	5	6	7	8	9	10
7	1	2	3	4	5	6	7	8	9	10
8	1	2	3	4	5	6	7	8	9	10
9	1	2	3	4	5	6	7	8	9	10
10	1	2	3	4	5	6	7	8	9	10

Iteration 8 ($j = 8$) :

	1	2	3	4	5	6	7	8	9	10
1	0	$-\infty$	$-\infty$	27	$-\infty$	20	13	16	15	16
2	14	0	12	21	19	20	19	19	19	19
3	$-\infty$	$-\infty$	0	$-\infty$	17	17	17	17	17	17
4	$-\infty$	$-\infty$	$-\infty$	0	$-\infty$	20	13	16	15	16
5	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	18	21	21	20	21
6	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	$-\infty$	16	15	16
7	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	22	20	22
8	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	14	26
9	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0	25
10	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	$-\infty$	0

	1	2	3	4	5	6	7	8	9	10
1	1	2	3	4	5	4	4	6	6	8
2	1	2	3	4	5	4	5	7	7	8
3	1	2	3	4	5	5	5	7	7	8
4	1	2	3	4	5	6	7	6	6	8
5	1	2	3	4	5	6	7	7	7	8
6	1	2	3	4	5	6	7	8	9	8
7	1	2	3	4	5	6	7	8	9	8
8	1	2	3	4	5	6	7	8	9	10
9	1	2	3	4	5	6	7	8	9	10
10	1	2	3	4	5	6	7	8	9	10

Iteration 9 ($j = 9$) :

$$\left[\begin{array}{c|cccccccccc}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
\hline
1 & 0 & -\infty & -\infty & 27 & -\infty & 20 & 13 & 16 & 15 & 16 \\
2 & 14 & 0 & 12 & 21 & 19 & 20 & 19 & 19 & 19 & 19 \\
3 & -\infty & -\infty & 0 & -\infty & 17 & 17 & 17 & 17 & 17 & 17 \\
4 & -\infty & -\infty & -\infty & 0 & -\infty & 20 & 13 & 16 & 15 & 16 \\
5 & -\infty & -\infty & -\infty & -\infty & 0 & 18 & 21 & 21 & 20 & 21 \\
6 & -\infty & -\infty & -\infty & -\infty & -\infty & 0 & -\infty & 16 & 15 & 16 \\
7 & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & 0 & 22 & 20 & 22 \\
8 & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & 0 & 14 & 26 \\
9 & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & 0 & 25 \\
10 & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & 0
\end{array}\right]$$

$$\left[\begin{array}{c|cccccccccc}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
\hline
1 & 1 & 2 & 3 & 4 & 5 & 4 & 4 & 6 & 6 & 8 \\
2 & 1 & 2 & 3 & 4 & 5 & 4 & 5 & 7 & 7 & 8 \\
3 & 1 & 2 & 3 & 4 & 5 & 5 & 5 & 7 & 7 & 8 \\
4 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 6 & 6 & 8 \\
5 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 7 & 7 & 8 \\
6 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 8 \\
7 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 8 \\
8 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
9 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
10 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10
\end{array}\right]$$

Iteration 10 ($j = 10$) : This is the final capacity and route matrices.

$$\left[\begin{array}{c|cccccccccc}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
\hline
1 & 0 & -\infty & -\infty & 27 & -\infty & 20 & 13 & 16 & 15 & 16 \\
2 & 14 & 0 & 12 & 21 & 19 & 20 & 19 & 19 & 19 & 19 \\
3 & -\infty & -\infty & 0 & -\infty & 17 & 17 & 17 & 17 & 17 & 17 \\
4 & -\infty & -\infty & -\infty & 0 & -\infty & 20 & 13 & 16 & 15 & 16 \\
5 & -\infty & -\infty & -\infty & -\infty & 0 & 18 & 21 & 21 & 20 & 21 \\
6 & -\infty & -\infty & -\infty & -\infty & -\infty & 0 & -\infty & 16 & 15 & 16 \\
7 & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & 0 & 22 & 20 & 22 \\
8 & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & 0 & 14 & 26 \\
9 & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & 0 & 25 \\
10 & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & -\infty & 0
\end{array}\right]$$

$$\left[\begin{array}{c|cccccccccc}
 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
\hline
1 & 1 & 2 & 3 & 4 & 5 & 4 & 4 & 6 & 6 & 8 \\
2 & 1 & 2 & 3 & 4 & 5 & 4 & 5 & 7 & 7 & 8 \\
3 & 1 & 2 & 3 & 4 & 5 & 5 & 5 & 7 & 7 & 8 \\
4 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 6 & 6 & 8 \\
5 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 7 & 7 & 8 \\
6 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 8 \\
7 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 8 \\
8 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
9 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
10 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10
\end{array}\right]$$

The max capacity chain is $2 \rightarrow 10$, with a length of 19. $r^*_{2,10} = 8, 2 \rightarrow 10$ via 8. $r^*_{8,10} = 10$, direct. $r^*_{2,8} = 7, 2 \rightarrow 8$ via 7. $r^*_{7,8} = 8$, direct. $r^*_{2,7} = 5, 2 \rightarrow 7$ via 5. $r^*_{5,7} = 7$ direct. $r^*_{2,5} = 5$ direct. The path is $2 \rightarrow 5 \rightarrow 7 \rightarrow 8 \rightarrow 10$.

(c) The min cut — to verify the max flow/min cut theorem.

Solution: Finding the min cut is not as simple as finding the max flow. In this network, one can eyeball it and see that the min cut contains arcs (8, 10) and (9, 10), but as the size of the network increase, eye balling the solution is not ideal. It is much easier to use the max flow algorithm we know also to be the min cut value. The min cut would include only arcs whose capacity was completely used during the max flow process, but usually not all of them — there are often ties. But reducing the number of arcs to consider to those whose capacity is filled helps immeasurably when find the min cut. However, given the problem to find the min cut in Figure 6.75 on page 394, I shall attempt to go about the process in some logical fashion.

First, I suspect the min cut to consist of arcs (8, 10) and (9, 10) for a total of 51. By testing all possible categories of sets of arc cuts, I shall show that 51 is the minimal cut through the network. By examination, we see the smallest value in the network is 12. For the time being, supposing there were more than one arc with a capacity of 12, we know we can only consider cut of 4 arcs or less since $5 \times 12 = 60 > 51$. So we shall consider each case.

Min cuts of two arcs: only one exists in the network, and it is the one we are using as our reference.

Min cuts of three arcs: again only one exists and it is (9, 10), (6, 8), and (7, 8) for a total of $63 > 51$.

Both min cuts of two and three arcs are fairly easy to see in any network because there will only be a minimal number of possible cuts to consider that will definitely obstruct the path. Min cuts of four are less easy t visualize as there are usually several possibilities to consider. So, the following logical deduction probes to be worthy. We know of a cut of 51 which we are trying to underscore if possible. $\frac{51}{4} = 12.75$, and 12 is the smallest arc capacity in the network. So, if there were a four arc min cut, it must contain arcs with capacities around 12.75. Let's allow arc (2, 3) with a capacity of 12 to be in our tentative min cut. We now must choose the remaining three arcs so that the capacities are no greater than $51 - 12 = 39$. $\frac{39}{3} = 13$, so the remaining three arcs will be around 13 (because 12 is the smallest arc capacity and if there were more than two arcs with capacity 12, we would have used them during the first step). By inspection, we see there is only one arc with a capacity between 12 and 13 and it is arc (4, 7) with a capacity of 13. So, the remaining two arcs must sum to $39 - 13 = 26$. $\frac{26}{2} = 13$, but there are no arcs left in the network to include that are less than or equal to 13. Consequently, there will not be a cut of four arcs less than 51.

We may now conclude that (8, 10), (9, 10) is the minimal cut with a value of 51. This number correlates with the maximum flow found in Part (a). Thus, verifying the max flow/min cut theorem. Obviously, the above method for finding the min cut is nowhere near ideal and allows great cause for errors. However, knowing the validity of the max flow/min cut theorem, allows one to use it to find the min cut through finding the max flow.

6. Problem 18, page 388 of the Hillier and Lieberman text. Use the transportation simplex method to solve the problem.

Solution: In this problem, we were asked to formulate the network representation of a transportation problem. The north west corner rule was used to obtain an initial feasible solution. Then, the transportation simplex method was used to solve the problem. A trace of the Hillier & Lieberman "OR

Course ware" follows.

```
Transportation Problem Model

Number of sources: 2
Number of destinations: 3

    Cost per unit distributed

       |  Destination    |
       |  1     2      3 | Supply
-------|-----------------|-------
      1|  6     7      4 | 40
      2|  5     8      6 | 60
-------|-----------------|-------
Demand | 30    40     30 |
       |                 |

Interactive Transportation Simplex Method


Key:
  B - A Basic Variable
  E - Entering Basic Variable
  L - Leaving Basic Variable
  P - A Basic Variable in Path


       |  Destination    |
       |  1     2      3 | Supply   u[i]
-------|-----------------|--------------
       |  6     7      4 |
      1|---B|---B|-------|         |
       |  30|  10|      0|       40|   0
       |----|----|-------|         |
       |   5|   8|      6|         |
      2|----|---B|------B|         |
       |   0|  30|     30|       60|   0
       |----|----|-------|---------|------
Demand |  30   40      30|
-------|-----------------|
  v[j] |   0    0       0|
       |                 | z = 670


       |  Destination    |
       |  1     2      3 | Supply   u[i]
-------|-----------------|--------------
       |  6     7      4 |
      1|---B|---B|-------|         |
       |  30|  10|      0|       40|   0
       |----|----|-------|         |
       |   5|   8|      6|         |
```

```
      2|----|---B|------B|         |
       |   0|  30|     30|      60|   1
       |----|----|-------|---------|------
Demand |  30   40      30|
-------|-----------------|
  v[j] |   0    7       4|
       |                 | z = 670


       |  Destination    |
       |  1     2      3 | Supply   u[i]
-------|-----------------|--------------
       |  6     7      4 |
      1|---B|---B|-------|         |
       |  30|  10|      0|      40|   0
       |----|----|-------|         |
       |   5|   8|      6|         |
      2|----|---B|------B|         |
       |   0|  30|     30|      60|   1
       |----|----|-------|---------|------
Demand |  30   40      30|
-------|-----------------|
  v[j] |   0    7       4|
       |                 | z = 670

       |  Destination    |
       |  1     2      3 | Supply   u[i]
-------|-----------------|--------------
       |  6     7      4 |
      1|---B|---B|-------|         |
       |  30|  10|      0|      40|   0
       |----|----|-------|         |
       |   5|   8|      6|         |
      2|----|---B|------B|         |
       |   0|  30|     30|      60|   1
       |----|----|-------|---------|------
Demand |  30   40      30|
-------|-----------------|
  v[j] |   0    7       4|
       |                 | z = 670


       |  Destination    |
       |  1     2      3 | Supply   u[i]
-------|-----------------|--------------
       |  6     7      4 |
      1|---B|---B|-------|         |
       |  30|  10|      0|      40|   1
       |----|----|-------|         |
       |   5|   8|      6|         |
      2|----|---B|------B|         |
       |   0|  30|     30|      60|    0
       |----|----|-------|---------|------
Demand |  30   40      30|
```

```
-------|-----------------|
  v[j] |   5    8       4|
       |                 | z = 670


       |  Destination    |
       |  1     2      3 | Supply   u[i]
-------|-----------------|--------------
       |  6     7      4 |
      1|---B|---B|-------|         |
       |  30|  10|      0|       40|   1
       |----|----|-------|         |
       |   5|   8|      6|         |
      2|----|---B|------B|         |
       |   0|  30|     30|       60|   0
       |----|----|-------|---------|------
Demand |  30   40      30|
-------|-----------------|
  v[j] |   5    8       4|
       |                 | z = 670


       |  Destination    |
       |  1     2      3 | Supply   u[i]
-------|-----------------|--------------
       |  6     7      4 |
      1|---B|---B|-------|         |
       |  30|  10|      0|       40|   1
       |----|----|-------|         |
       |   5|   8|      6|         |
      2|----|---B|------B|         |
       |   0|  30|     30|       60|   0
       |----|----|-------|---------|------
Demand |  30   40      30|
-------|-----------------|
  v[j] |   5    8       4|
       |                 | z = 670


       |  Destination    |
       |  1     2      3 | Supply   u[i]
-------|-----------------|--------------
       |  6     7      4 |
      1|---L|---P|-------|         |
       |  30|  10|      0|       40|  -1
       |----|----|-------|         |
       |   5|   8|      6|         |
      2|---E|---P|------B|         |
       |  -2|  30|     30|       60|   0
       |----|----|-------|---------|------
Demand |  30   40      30|
-------|-----------------|
  v[j] |   7    8       6|
       |                 | z = 670
```

```
       |  Destination    |
       |  1     2      3 | Supply   u[i]
-------|-----------------|--------------
       |  6     7      4 |
      1|--- |---P|------E|         |
       |   2|  40|     -1|       40|  -1
       |----|----|-------|         |
       |   5|   8|      6|         |
      2|---B|---P|------L|         |
       |  30|   0|     30|       60|   0
       |----|----|-------|---------|------
Demand |  30   40      30|
-------|-----------------|
  v[j] |   5    8       6|
       |                 | z = 610
```

```
       |  Destination    |
       |  1     2      3 | Supply   u[i]
-------|-----------------|--------------
       |  6     7      4 |
      1|--- |---B|------B|         |
       |   2|  10|     30|       40|   0
       |----|----|-------|         |
       |   5|   8|      6|         |
      2|---B|---B|------ |         |
       |  30|  30|      1|       60|   1
       |----|----|-------|---------|------
Demand |  30   40      30|
-------|-----------------|
  v[j] |   4    7       4|
       |                 | z = 580
```

7. Problem 15, page 388 of Hillier and Lieberman. Solve with dynamic programming, not the network simplex algorithm. Solution: We were asked to formulate a shortest path problem as a network problem and solve using dynamic programming.

   A small growing airline company is purchasing a tractor to carry luggage to and from their aircrafts. In three years time, the company plans to install a mechanized system for transporting luggage but must use the tractor in the mean time. The company may decide to replace the tractor after one or two years time if they feel it would be more economical due to the maintenance and aging of the tractor. We must help hem decide if and when they should replace the current tractor with a new one. The following table contains the net discounted cost (purchase price minus trade in allowance, plus running and maintenance costs) for buying in year i (row) and selling in year j (column).

Year	1	2	3
0	8	18	31
1	–	10	21
2	–	–	12

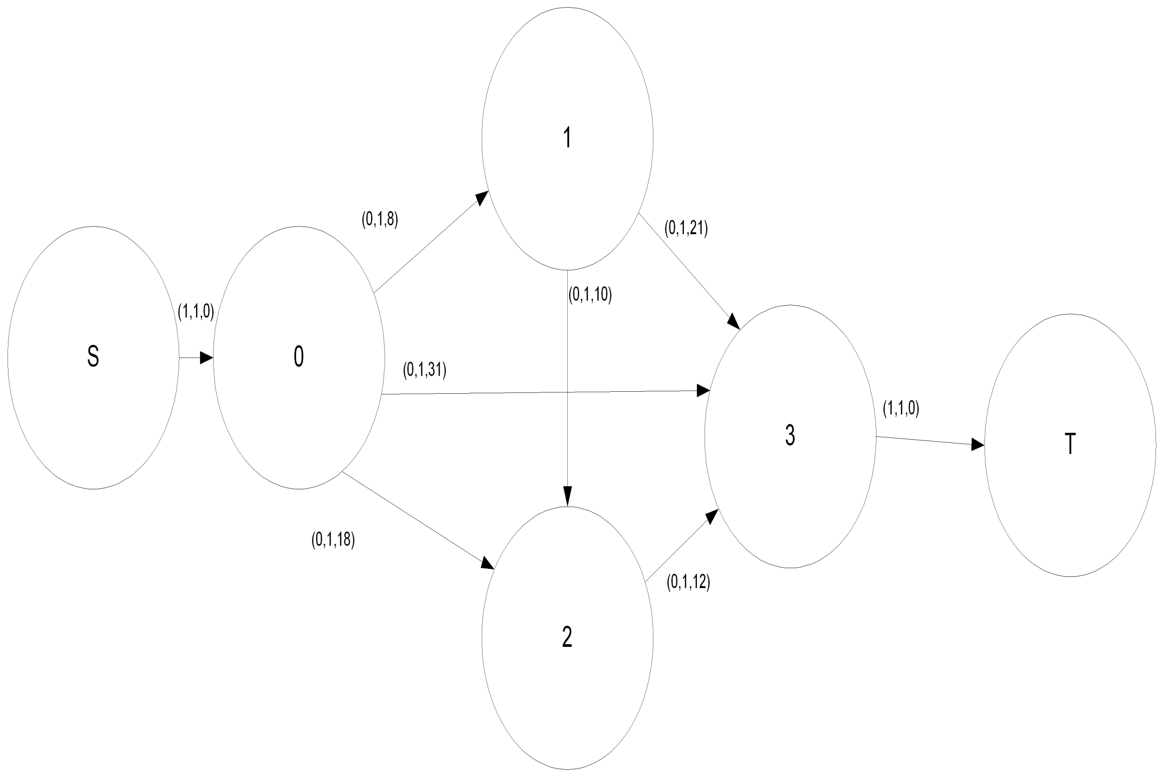

Figure 6.77: *This figure shows the shortest path problem as a network problem.*

Formulating the problem as a shortest path problem is quite easy, but drawing the network as a MCNFP is tricky. I toiled with several ideas for the network and was unable to come up with one that completely satisfied me. My problem arose when trying to represent the cost. Because of the nonlinearity of costs from selling or carrying over, the problem became somewhat like the turn penalty problem where a person could be under charged for a certain route one way or over charged for a certain route another way. The best network I could design is depicted in Figure 6.77 where the arcs represent $(L_{ij}, U_{ij}, cost)$. The network seems little different than the shortest path network. An arc leads from the source node to year 0 node with $L_{ij} = 1$ to ensure that at least one tractor passes through the network. This requirement in reality has been taken care of since we know they have already purchased a tractor at year 0, but we cannot represent this lower bound without introducing a dummy source node. U_{ij} is also 1 since only one tractor moves through the network. More than one tractor can be purchased but only if the prior one is sold. Consequently, the upper bound entering the network is 1. A dummy terminal node is also added, although in reality year 3 is the final year. Placing an arc from 3 to t ensures that at least one tractor passes through the network. The dummy source and dummy terminal both account for the same problem, but having both present in the network allows more generality so possible future changes can be easily incorporated. The rest of the network is fairly straightforward using the variables for the MCNFP ad defined as follows: x_{ij} is equal to 0 or 1; in reality; if $x_{ij} = 1$ then a tractor bought in year i was sold in year j. Because x_{ij} can only be an integer, dynamic programming is an appropriate method to use to solve the problem. $U_{ij} = 1$ is the upper-bound of the variable x_{ij}. $L_{ij} = 0$ is the lower bound of variable x_{ij}. c_{ij} is the cost to sell in year j given it was bought in year i. $b_{ij} = 1, -1, 0$. This value is not really apparent in the network, rather it is incorporated in the upper/lower bound value, where a -1 corresponds to a lower bound value of 1. The following matrix utilizes all of the variables and non-pictorially describes the MCNFP.

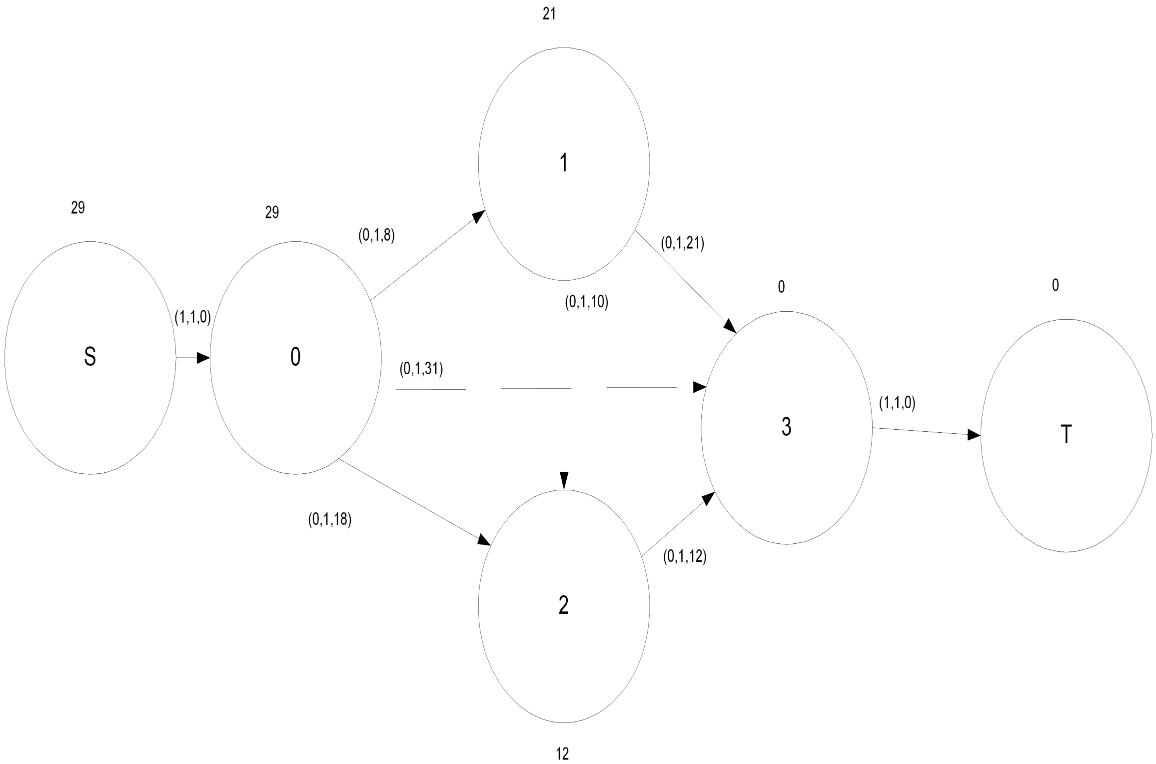

Figure 6.78: *This figure shows the solution to the dynamic programming problem.*

$$\min \left[\begin{array}{cccccc} x_{01} & x_{02} & x_{03} & x_{12} & x_{13} & x_{23} \\ \hline 8 & 18 & 31 & 10 & 21 & 12 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 1 & 0 \\ 0 & -1 & 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 0 & -1 & -1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right] \begin{array}{cc} = & 1 \\ = & 0 \\ = & 0 \\ = & -1 \\ \leq & 1 \\ \leq & 1 \\ \leq & 1 \\ \leq & 1 \\ \leq & 1 \\ \leq & 1 \end{array}$$

For all variables greater-than or equal to 0, i.e. $L_{ij} = 0$. Figure 6.78 on page 407 depicts the network after solving using dynamic programming. The values on top or underneath the nodes that were applied during the process of tracing backwards through the network. We see that the optimal path is $S \to 0 \to 1 \to 3 \to T$. Meaning, we should sell the first tractor at year 0 and purchase a new one. The second tractor shall be used for the remainder of the time period.

8. Problem 14, page 387 of Hillier and Lieberman. Omit part (d).

   Solution: A company is producing the same product in two factories to be distributed according to demand to two warehouses. Factory $1- > 2$ may ship unlimited quantities to warehouse $1- > 2$ but cannot ship to warehouse $2- > 1$ directly. A distribution center is located between the factories and warehouses. Each factory can ship upto the 50 units to the distribution center; from there the distribution center can ship up to 50 units to either warehouse. The shipping costs per unit along with the supply and demand amounts can be read in the following table.

	Dist. Center	Ware. 1	Ware. 2	Supply
Fact. 1	3	7	–	80
Fact. 2	4	–	9	70
Dist. Ctr.		2	4	
Demand		60	90	

(a) Formulate a network as a MCNFP. Solution: In Figure 6.79, the F_i, W_i, and D nodes represent the factories, warehouses, and distribution center respectively. The variables of a MCNFP drawn in the network can be defined as follows: x_{ij} is the amount shipped along arc (i, j); U_{ij} is the capacity/supply (upper bound) of arc (i, j); $L_{ij} = 0$ is the 0/demand (lower bound) of arc (i, j); c_{ij} is the cost to ship one unit along arc (i, j). For writing the LP to the problem, the variable b_{ij} can be defined as follow: b_{ij} is the (supply, demand, 0) for (source, destination, intermediate). But, in the network drawing, b_{ij} is included in the U_{ij} and L_{ij} because there were no arcs that had both capacity and supply/demand amounts applied to it. The labels in the network represent $(L_{ij}, U_{ij}, \text{cost/unit})$. Note that once supply or demand is accounted for on one arc, it need not be represented on other arcs. This allows the problem to be more general and easier to change later if necessary. For example, the arc from Factory 1 to Warehouse 1 shows capacity as being infinite, when in reality, the amount able to be shipped along that arc is no greater than 80, or the supply of Factory 1. But this constraint is taken care of on the arc entering Factory 1. If no more than 80 can get into Factory 1, obviously, no more than 80 will come out of it regardless of what capacity amounts we place on the arcs out of Factory 1.

(b) Formulate the LP for this model. Solution: Let the variables be defined similarly as in Part (a). x_{ij} is the amount shipped from node i (Factory 1, 2; distance D); U_{ij} is the upper bound (capacity) of variable x_{ij}; L_{ij} is the lower bound (0) of variable x_{ij}; c_{ij} is the cost to ship one unit of x_{ij} or the coefficient of x_{ij} in the objective function; b_{ij} is the (supply, demand, 0) for (source, destination, intermediate). The LP becomes.

$$\min 7x_{11} + 3x_{1D} + 2x_{D1} + 4x_{2D} + 4x_{D2} + 9x_{22}$$

subject to

$$\begin{array}{l|r}
x_{11} + x_{1D} \leq 80 & \text{Supply Factory 1} \\
x_{22} + x_{2D} \leq 70 & \text{Supply Factory 2} \\
x_{11} + x_{D1} \geq 60 & \text{Demand Warehouse 1} \\
x_{22} + x_{D2} \geq 90 & \text{Demand Warehouse 2} \\
x_{1D} + x_{2D} + x_{D1} + x_{D2} = 0 & \text{In=Out, Distribution Center} \\
x_{1D} \leq 50 & \\
x_{2D} \leq 50 & \\
x_{D1} \leq 50 & \\
x_{D2} \leq 50 &
\end{array}$$

The supply and demand constraints are expressed as inequalities instead of equalities as it is easier for LINDO to solve equations of the former type. Since supply equals demand, the solution LINDO prints out will force the equations to become equalities. The next table shows the LINDO output for the problem. The solution dictates that the company should ship 30 units directly from Factory 1 to Warehouse 1 and 50 units to the distribution center. 40 units should be shipped directly from Factory 2 to Warehouse 2 and 30 units to the distribution center. From the distribution center, 30 and 50 units are to be shipped to Warehouse 1 and 2 respectively. The total cost is \$1,100.

```
MIN     7 X11 + 3 X1D + 2 XD1 + 4 X2D + 4 XD2 + 9 X22

SUBJECT TO
       2)   X11 + X1D <=   80
       3)   X2D + X22 <=   70
       4)   X11 + XD1 >=   60
       5)   XD2 + X22 >=   90
       6)   X1D - XD1 + X2D - XD2 =     0
       7)   X1D <=   50
       8)   X2D <=   50
       9)   XD1 <=   50
      10)   XD2 <=   50

:  LP OPTIMUM FOUND AT STEP     8

       OBJECTIVE FUNCTION VALUE

       1)   1100.00000

VARIABLE         VALUE          REDUCED COST
     X11         30.000000           .000000
     X1D         50.000000           .000000
     XD1         30.000000           .000000
     X2D         30.000000           .000000
     XD2         50.000000           .000000
     X22         40.000000           .000000


     ROW    SLACK OR SURPLUS     DUAL PRICES
      2)           .000000           .000000
      3)           .000000          1.000000
      4)           .000000         -7.000000
      5)           .000000        -10.000000
      6)           .000000         -5.000000
      7)           .000000          2.000000
      8)         20.000000           .000000
      9)         20.000000           .000000
     10)           .000000          1.000000

NO. ITERATIONS         8
```

(c) Obtain an initial basic feasible solution using the feasible spanning tree that corresponds to using the two direct shipping lines with Factory 1 shipping to Warehouse 2 via the distribution center. Solution: Figure 6.80 depicts the spanning tree described above; the source and terminal nodes have been eliminated and replaced by arcs entering/leaving the factories/warehouses. Since Factory 2 has a supply of 70 and Warehouse 2 has a demand of 90, 20 units must be shipped from Factory 1 to Warehouse 2 via the distribution center. Factory 1 can send no more than 20 units to Warehouse 2 because it needs 60 units of its supply to send to Warehouse 1. The labels in Figure 6.80 represent (amount sent, cost/unit). The initial basic feasible solution has a cost of $1,190.

9. During the next three months, Shoemakers, Inc. must meet (on time) the following demands for shoes: month 1, 1000 pairs; month 2, 1500 pairs; months 3, 1800 pairs. It takes 1 hour of labor to produce a pair of shoes. During each of the next three months, the following number of regular-time labor hours are available: month 1, 1000 hours; month 2, 1200 hours; month 3, 1200 hours. Each month,

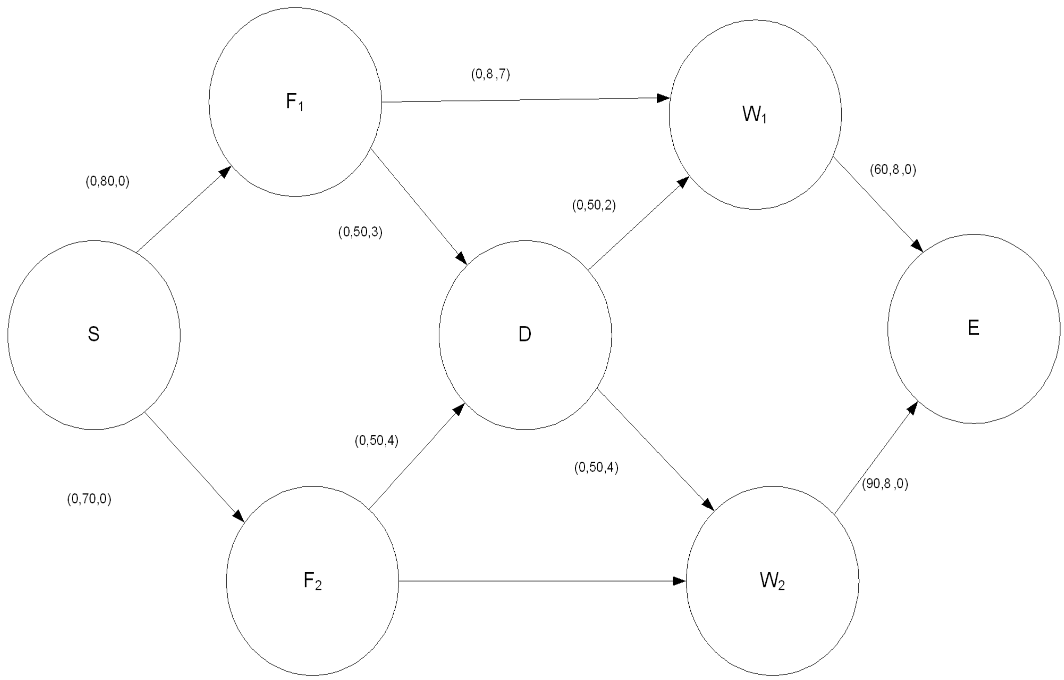

Figure 6.79: *This figure shows the factories, warehouses, and distribution center as an MCNFP problem.*

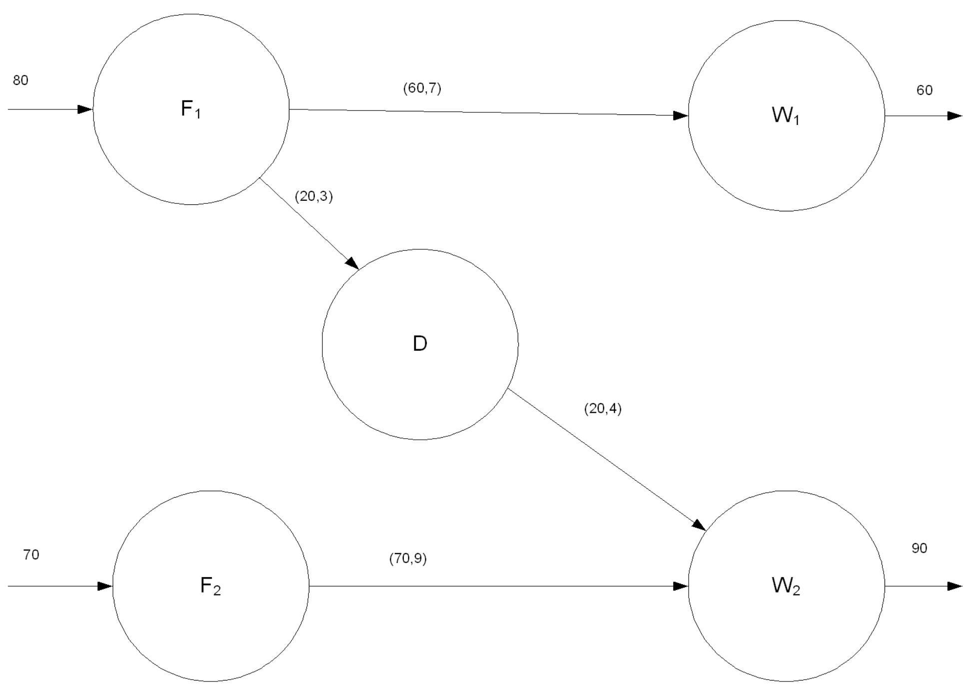

Figure 6.80: *This figure shows the spanning tree for the MCNFP problem.*

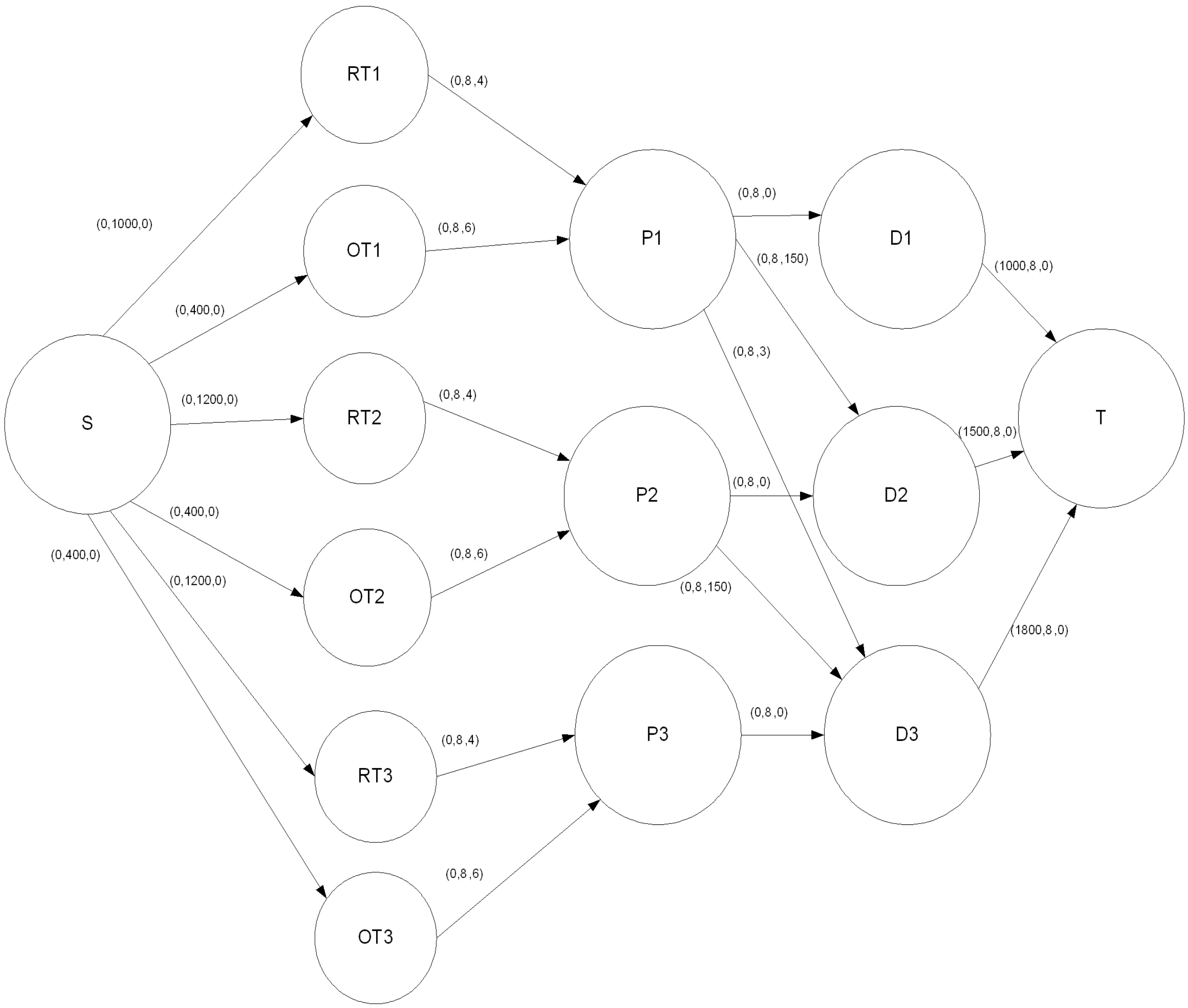

Figure 6.81: *The Shoemaker graph.*

the company can require workers to put in up to 400 hours of overtime. Workers are only paid for the hours they work, and a worker receives \$4 per hour for regular-time work and \$6 per hour for overtime work. At the end of each month, a holding cost of \$1.50 per pair of shoes is incurred. Formulate a MCNFP that can be used to minimize the total cost incurred in meeting the demands of the next three months. A formulation requires drawing the appropriate network and determining the c'_{ij}s and b'_js and arc capacities. How would you modify your answer if demand could be back-loaded (all demand must still be met by the end of month 3) at a cost of \$20/pair/month? Note: MCNFP means minimum cost network flow problem.

Solution: During the next 3 months, Shoemakers, Inc. must fulfill demands for pairs of shoes while adhering to their labor hour restrictions. The laborers can work both regular time (RT) and overtime (OT) hours each month. The following table summarizes the demand in pairs of shoes, available hours of RT and OT labor, and cost (wages) in dollars/hour for RT and OT labor.

Month	Demand	RT Hours	OT Hours	RT Wage	OT Wage
1	1000	1000	400	4	6
2	1500	1200	400	4	6
3	1800	1200	400	4	6

Shoemakers can produce ahead of time but incur a holding cost of \$1.50/pair/month. Each pair of shoes requires 1 hour of labor. Formulate a MCNFP to determine an optimal production schedule that minimizes cost while meeting demand.

Because the demand is represented in pairs of shoes but the hour restriction is represented in time, a manipulation of numbers may be needed. However, in this case, the amount of time required to produce a pair of shoes is 1, so the units of demand and units of supply carry a 1-1 correlation. If the numbers were changed in the future, it may become necessary to translate one unit in terms of the other in order to properly represent the lower and upper bounds in the network.

Let the variable of the MCNFP be defined as follows. x_{ij} is the number of pairs of shoes traveling along arc (i, j) Obviously, "traveling" means something different at each stage. It could represent the amount held over, or the amount sold in the same month as it is produced, etc. U_{ij} is the supply (upper bound) of time/pairs of shoes of arc (i, j). L_{ij} is the demand (lower bound) of pairs of node i to node j. c_{ij} is the cost of moving 1 unit from node i to node j — again the term "moving" carries different meanings depending on which two nodes are involved. For example it could be hourly wages, holding costs, etc. b_{ij} is the supply/demand for nodes — incorporated in L_{ij} and U_{ij}.

Figure 6.81 shows the network used for the MCNFP where the arc labels are $(L_{ij}, U_{ij}, cost)$. The network's node and arc meanings are as follow. S is the source. RT_i and OT_i are the source feeds the RT and OT nodes the number of allowable hours of labor — lower bound of 0 to allow for no hours to be used on a particular arc but ensure negative hours are not used, upper bound greater than 0 where the numbers represent values read from the table of information, cost of 0 as it costs nothing to "supply" the hours. P_i represents the shoes having just been produced and being temporarily held for selling distribution. RT_i and $OT_i \to P_i$ represents producing the shoes — lower bound of 0 to allow no production of shoes but not negative production, upper bound of infinity to make the problem more general. In reality, no more shoes can pass along the arc as can be produced according to the time restrictions, but using infinity as an upper bound allows for generality. A cost greater than 0 represents the wages of RT and OT hours. D_i denotes the product has just been sold to fulfill the demand for month i. $P_i \to D_i$ represents selling the shoes. It has a lower bound of 0 and upper bound of infinity for analogous reasons as stated earlier. The cost is greater than or equal to 0 where if the product is sold within the same month it is produced, the cost is 0 since there is no shipping cost. But, if the product is held over for a later month, the cost is (holding cost/month, or\$1.50)×(# months held over). T is the terminal node. $D_i \to T$ represents leaving the network. The lower bound is greater than 0 which equals the monthly demand. The upper bound is infinity. The cost of 0 has no shipping cost or other types of cost incurred.

The problem is now ready to be solved using the MCNFP algorithm. We are asked to suppose that demand for shoes may be back logged, or produced in a month after the month requiring them, as long as all demand is met by the end of month 3. Back logging orders would incur a cost of \$2.00/pair/month. How would adding this freedom affect the problem? Since orders can now be produced after the month in which they are demanded, arcs can be added so that every P_i node is attached to every D_i node. For late production, a cost of \$2.00 will be added to the arcs for every pair of shoes that travel along it. Figure 6.82 shows the network with this addition. All variables and arc movements are defined the same. Only there is greater freedom concerning meeting the monthly demands. Of course, using this greater freedom brings about a higher cost — quite similar to bouncing checks. But if the monthly

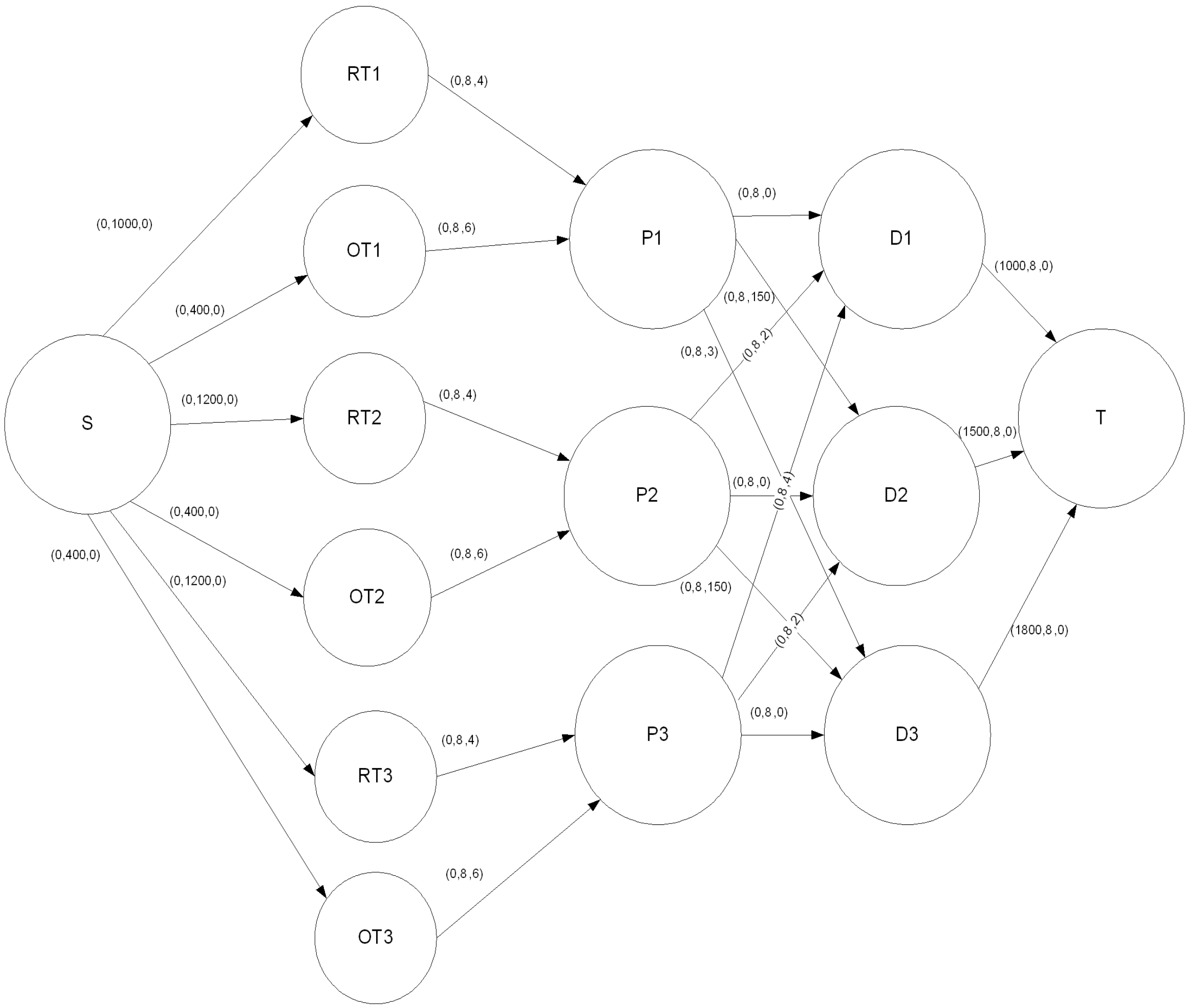

Figure 6.82: *The solution to the Shoemaker graph.*

hour restrictions are unable to meet the monthly demands without using later months to help out, then the Back logging allows demand to be met. Since the question posed stated that all months demands must be met by the end of month 3, no arcs representing production later than month 3 can enter the D_i nodes. Arcs cannot enter nodes D_i emanating from nodes that do not exist in the network. Also, the lower bound from D_3 to the terminal node must still be strictly followed.

10. State University has three professors who each teach four courses per year. Each year, four section of Marketing, Finance, and Production must be offered. At least one section of each class must be offered during each semester (Fall and Spring). Each professor's time preference and preference for teaching various courses are given in the following table.

	Prof 1	Prof 2	Prof 3
Fall preference	3	5	4
Spring preference	4	3	4
Marketing	6	4	5
Finance	5	6	4
Production	4	5	6

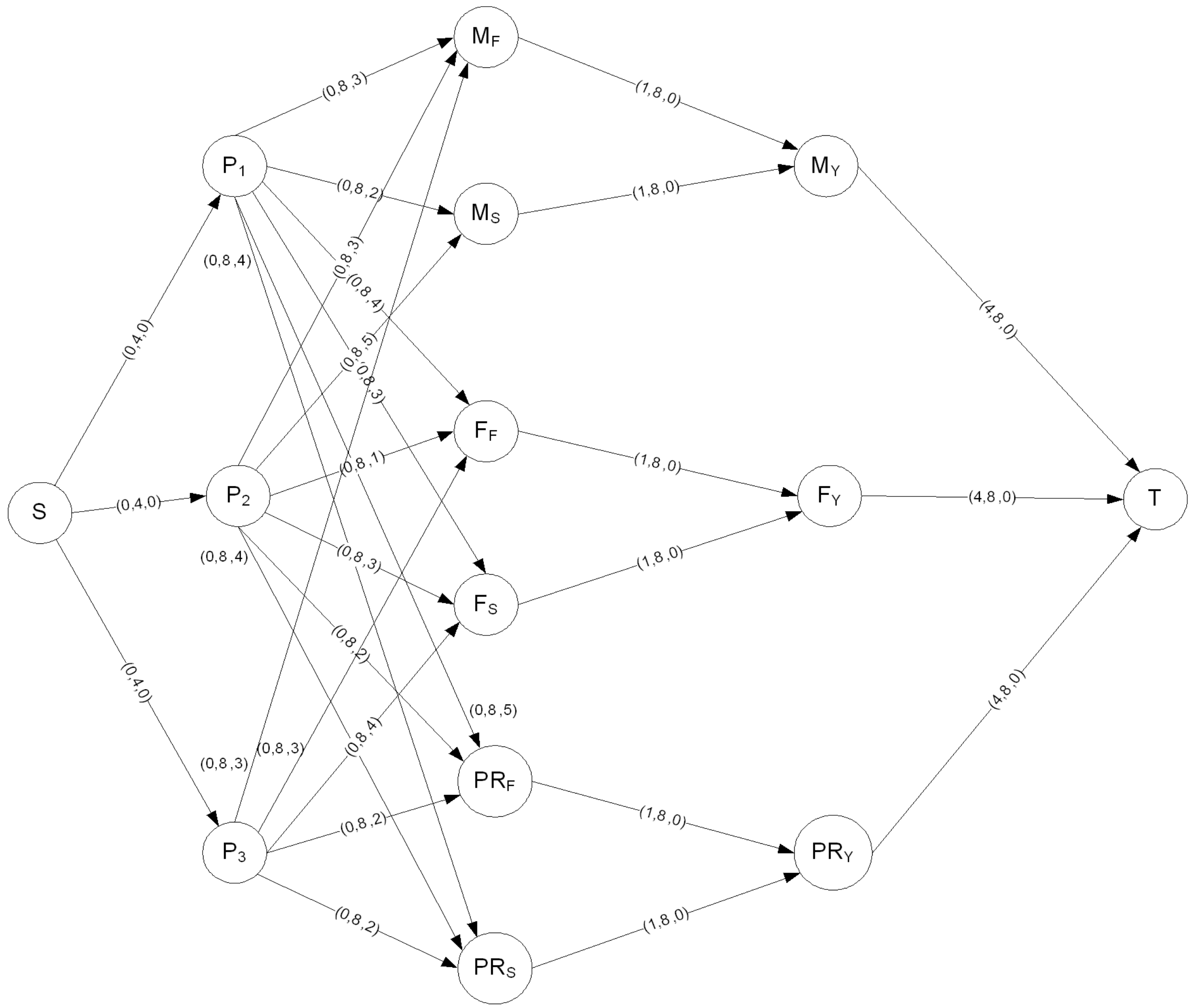

Figure 6.83: *The scheduling of professors problem.*

The total satisfaction a professor earns teaching a class is the sum of the semester satisfaction and the course satisfaction. Thus, professor 1 derives a satisfaction of $3 + 6 = 9$ from teaching marketing during the fall semester. Formulate an MCNFP that can be used to assign professors to courses so as to maximize the total satisfaction of the three professors.

Solution: State University needs to produce a class schedule for three professors with each professor teaching four courses per year. The courses offered are Marketing, Finance, and Production. Four sections of each must be offered and at least one of those sections must be offered in the fall and spring semester. The professors have ranked both the courses and time of year to teach according to personal preference, and the results are tabulized below.

Preferences Time:	Professor 1	2	3
Fall	3	5	4
Spring	4	3	4
Class:			
Marketing	6	4	5
Finance	5	6	4
Production	4	5	6

The University takes these two preferences and adds the numbers to attain a "satisfaction" factor. For example, professor 1 has a satisfaction factor of $3 + 6 = 9$ for teaching Marketing in the fall semester. Use the given information to formulate a MCNFP to produce a course schedule that maximizes the satisfaction factor of the professors.

Since the objective function desired is a maximum, and the MCNFP denotes a minimum objective function, we must first transform the preferences. If we take the highest preference number, although any number greater than or equal to the highest preference number will suffice, then subtract off each of the preferences, we obtain a table of "regret" preferences. By minimizing the regret factor, we will be maximizing the satisfaction factor. The table of regret preferences is as follows.

Preferences Time:	Professor 1	2	3
Fall	3	1	2
Spring	2	3	2
Class:			
Marketing	0	2	1
Finance	1	0	2
Production	2	1	0

The regret factor can be found by adding the two corresponding regret preferences. These numbers seem to be fairly straightforward, so I do not show the computations involved in getting them. Once the optimal schedule is known, the satisfaction factors can be easily attained either from the first table or by taking the regret factor and subtracting it from $12 = 6 + 6$. We must use 12 because two preferences (which we add) have been adjusted. Figure 6.84 shows the network for the scheduling problem. x_{ij}, U_{ij}, L_{ij} and c_{ij} are defined analogously to those in the previous problems. Again, b_{ij} is incorporated into L_{ij} and U_{ij}. The arc and node variables in the network are defined as follow. S is the source node. P_i is professor i. $S \to P_i$ represents the source allocating 4 courses to each professor as an upper bound. In this problem, because the total number of courses required to be offered equals the summed number of courses the professors are willing to teach, the lower bound could be 4 too. But, I made the lower bound be 0 to allow for more generality. The cost is 0. M_j, F_j, PR_j for $j = F, S$ these nodes represent the fall (F) or spring (S) offering of marketing (M), finance (F), and production (PR). $P_i \to M/F/P_j$ arcs indicate that professor i teaches course M/F/P in the fall/spring for $j = F/S$. The lower bound is 0 when the professor need not teach a particular $M/F/P_i$ course. The upper bound could have been 3 because a maximum of 3 courses of the same type can be taught per semester to allocate the requirement that at least one course per semester to be fulfilled for the second semester. However, the lower bounds of 1 on each arc take care of the possible upper bound problem.

Consequently, the upper bound is set at infinity for generality. The cost is the regret factor. Note that this arc is the only place in the network where a true cost is incurred. $M/F/P_i$ represents the course M/F/P for the year. $M/F/P_j \rightarrow M/F/P_j$ represents the accumulation of the semester requirements into the year requirements. This arc is the main reason why we required 3 nodes for the courses — two for the different semesters and one for the year. The lower bound is 1 because each course has a demand of 1 for both the fall and spring. The upper bound is infinity to make the problem more general, and the cost is 0. T is the terminal node. It represents the end of the year $M/F/P_j \rightarrow T$. The arc carries the yearly requirement of 4 sections of each course and represents leaving the network. The lower bound on all arcs is 4. The upper bound is infinity, and the cost is 0.

With the variables defined above, the network is fairly easy to follow. The MCNFP algorithm can be used to find an optimal course scheduling assignment and the total satisfaction factor can be attained by re-manipulating the numbers. The individual satisfaction total can be found by multiplying the number of different classes taught (i.e. M_f is not the same as M_s) by their corresponding satisfaction factor for each professor separately. Summing all relevant multiplicative totals will yield each faculty members' optimal (in light of the whole problem with the other two professors requirements added) satisfaction factor total.

11. During the next two months, Shoemakers, Inc must meet (on time) the following demands for three types of products shown in the following table. Two machines are available to produce these products. Machine 1 can only produce products 1 and 2, and machine 2 can only produce products 2 and 3. Each machine can be used for up to 40 hours per month. The table show the time required to produce 1 unit of each product (independent of the type of machine); the cost of producing 1 unit of each product on each type of machine; and the cost of holding 1 unit of each product in inventory for one month. Formulate an MCNFP that could be used to minimize the total cost of meeting all demands on time.

	Product 1	Product 2	Product 3
Month 1	50 units	70 units	80 units
Month 2	60 units	90 units	120 units

	Production Time	Production Cost Machine 1	Production Cost Machine 2	Holding Cost
Product 1	30	\$40	—	\$15
Product 2	20	\$45	\$60	\$10
Product 3	15	—	\$55	\$5

Solution: Shoemaker must meet demands over the next two months for three types of products. There are two machines available to make these products, but machine 1 can only produce products 1 and 2. Machine 2 can only produce products 2 and 3. Each machine can be used up to 40 hours per month. Additionally, the company can make products in month 1 and hold them in inventory for month 2 at a hold cost per unit. The tables carry the following relevant information concerning the three products: the required machine time per unit (independent of machine used), cost per unit incurred to produce with machine 1, the cost per unit incurred to produce with machine 2, the holding cost per unit per month, the month 1 demands (M1), and the month 2 demands (M2). Formulate an MCNFP to help Shoemaker determine the optimal production schedule.

The variables x_{ij}, U_{ij}, L_{ij} and c_{ij} are defined as they were in the previous problems. Again, b_{ij} is incorporated into L_{ij} and U_{ij}. However, assigning numbers to the lower and upper bounds is tricky. The data presented restricts the machine use (U_{ij}) in time units, but the demand (L_{ij}) is in production units. Consequently, some manipulation of the numbers is required. Problem 9 had a similar case where time and units were mixed. However, in that problem, it took exactly 1 hour to make 1 pair of shoes. So, although the units were different, the correlation between the units was 1-1 and no manipulation was needed. I chose to represent the demand as time units, although it would have been equally easy and correct to represent the

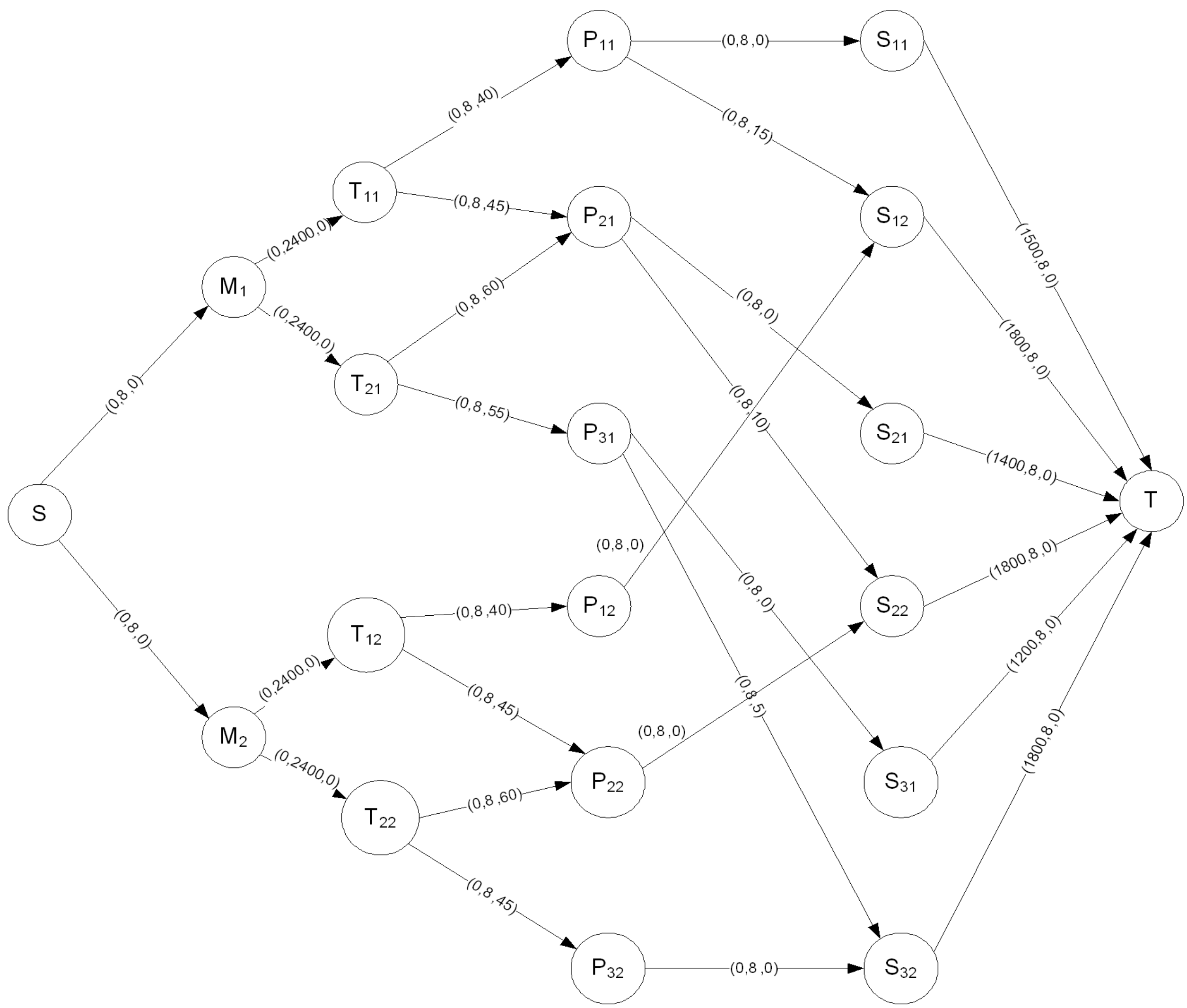

Figure 6.84: *The Shoemaker problem, again.*

time restriction in terms of product units. The demands, therefore, become(unit demand) $\times$ (minutes of machine time required).

Product	$M1$	$M2$
1	$50 \times 30 = 1500$	$60 \times 30 = 1800$
2	$70 \times 20 = 1400$	$90 \times 20 = 1800$
3	$80 \times 15 = 1200$	$120 \times 15 = 1800$

Figure 6.84 depicts the network used for formulating this problem as an MCNFP. The arcs represent $(L_{ij}, U_{ij}, cost)$, and the following notation describes the node names and activity represented on the arcs with the placement of bounds or costs.

S is the source node. M_j is month j. $S \to M_j$ is the total time allocation for month j. The lower bound is 0. We need not use any time units if desired, but let's use infinity to make the problem more general. The true upper bound restriction is represented on later arcs. The cost of 0 as time costs nothing. T_{ij} is the time form machine i used in month j. $M_j \to T_{ij}$ is the time allocated in month j to machine i. The lower bound is 0 for the same reasoning. The upper bound is 2400 which is the number of possible allocated minutes. The costs of 0 is for P_{kj}, for product k made in month j. $T_{ij} \to P_{kj}$ is the arc producing product k in month j by machine i. The lower bound is 0. We cannot produce negative products, but we can produce 0 products. The upper bound is infinity for generality. The cost is greater than 0 and follows the table information. $_{kj}$ is the sold product k which was produced in month j. $P_{kj} \to S_{kj}$ represents the process of selling product k, made in month j, where the two notational j's may differ. The lower bound is 0. The upper bound is infinity. The cost equals 0 if the notational j's are the same or the cost is equal to 15 which is equal to the holding cost if the notational j's differ. T is the super terminal. $S_{kj} \to T$ represents departing the network. The lower bound is greater than 0. The upper bound is infinity. The cost is 0.

As described above, all costs, demands, and restrictions are only represented once in the network to preserve generality and ease of possible future change. Note that no arc attaches machine 1 to product 3 — as machine 1 cannot produce product 3. Similarly, no arc attaches machine 2 to product 1. The network is ready to be solved using the MCNFP algorithm.

6.13 The Transportation Problem

For the transportation problem read Section 2.0 of the text book. The transportation problem can be formulated as:

1. An LP formulation. We want to minimize $\sum_i \sum_j c_{ij} x_{ij} = z$ subject to $\sum_j x_{ij} = a_i$. This is the source constraint. And subject to $\sum_j x_{ij} = b_j$. This is the destination constraint. The equalities can be replaced with less-than or equal and greater-than or equal signs. The final condition is $x_{ij} \geq 0$.

2. A network formulation. See Figure 6.85. S and T are dummy source and destinations. We must send a_{51} from S to T over one or more $b_1, b_2, b_3, ...$ If $\sum_i a_i \neq \sum_j b_j$, then add dummy sources and destinations. If $\sum a_i = 120$ and $\sum_j b_j = 100$, then add to the destination 20. Note if c_{ij} represents profits, you can negate c_{ij} and then minimize.

   Example: Consider the following table. Use the northwest corner method for finding a feasible solution.

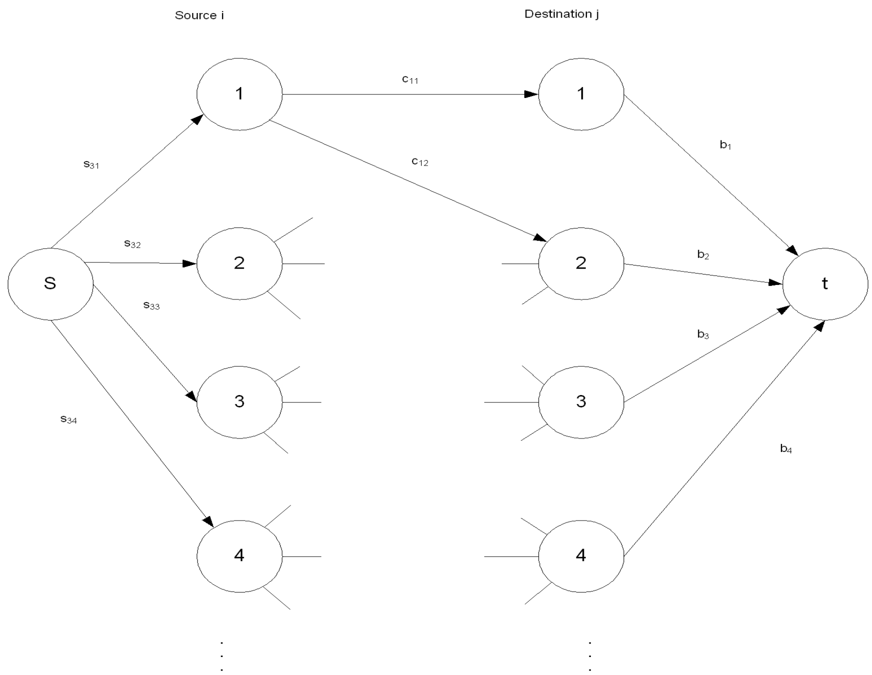

Figure 6.85: An example of a transshipment problem.

	1	2	3	4	
1	8	6	10	9	37
2	9	2	3	7	50
3	14	9	16	5	40
	45	22	30	30	127

After applying the northwest corner method, we have the following table. Note: the reader should not confuse the column and row totals as zero as addition. These are simply terminal calculations.

	1	2	3	4	
1	37				0
2	8	22	30		0
3			10	30	0
	0	0	0	0	

$z = 1202$.

6.13.1 Transportation Simplex Method

The transportation simplex method is an easy version of the simplex method. This method is performed right on the table (grid). Start with a feasible solution, choose an entering variable, reduce another variable to 0 (this is the pivot step), and adjust all other floats. Using the example in the previous section, the optimal solution is $z = 1032$. $x_{12} = 12, x_{13} = 25, x_{21} = 45, x_{22} = 5, x_{32} = 10, x_{34} = 3$.

Consider the transshipment problem. Refer to Section 2.11 in the text book. Stated as an LP problem, minimize $z = \sum_i \sum_j c_{ij}x_{ij} + \sum_i \sum_k c_{ik}x_{ik} + \sum_k \sum_j c_{kj}x_{kj}$ subject to the following constraints.

$$\sum_j x_{ij} = a_i,$$

$$\sum_i x_{ik} = \sum_j x_{kj},$$

$$\sum_i x_{ij} = b_j,$$

$$x_{ij} \geq 0.$$

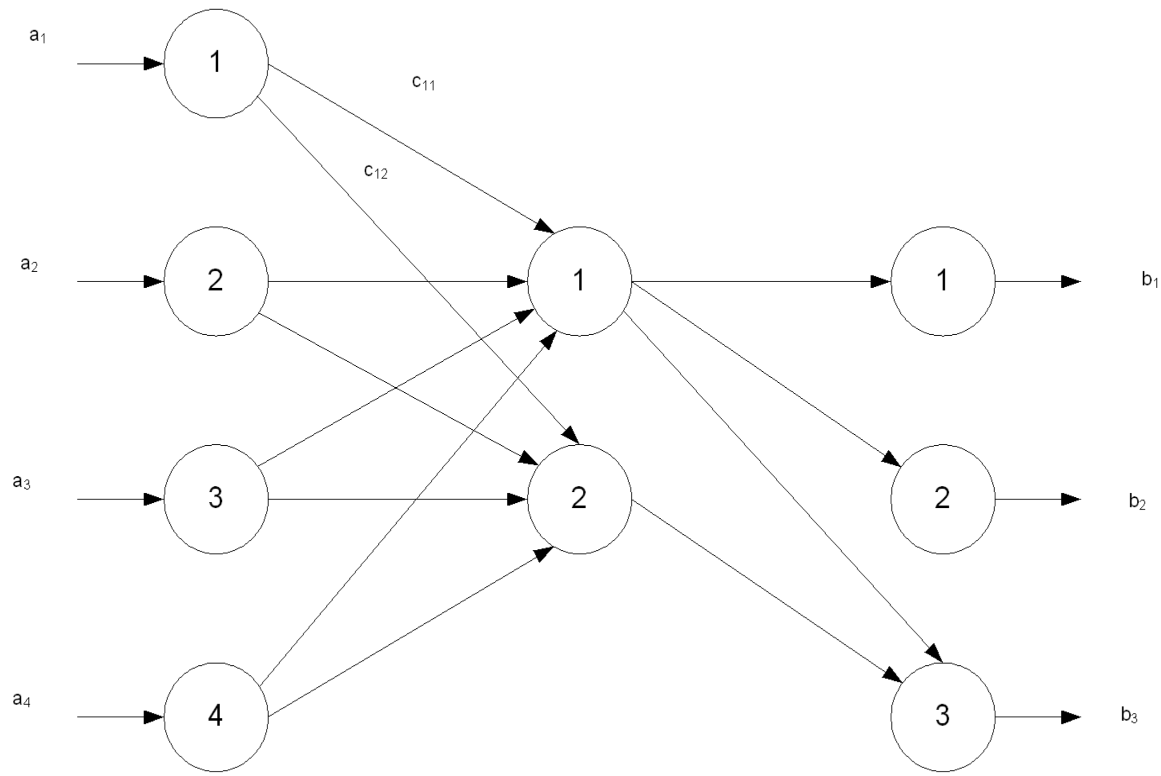

Figure 6.86: A transshipment problem.

The network sources in Figure 6.86 are i. k is the transshipment.
Now consider the transshipment problem in Figure 6.87. The LP formulation of the problem is min$[Ax + 2Ay + 3Bx + By + 2Bz + 5x_1 + 7x_2 + 9y_1 + 6y_2 + 7y_3 + 8z_2 + 7z_3 + 4z_4]$ subject to the constraints,

$$Ax + Ay = 9,$$

$$Bx + By + Bz = 8,$$

$$-Ax - Bx + x_1 + x_2 = 0,$$

$$-Ay - By + y_1 + y_2 + y_3 = 0,$$

$$-Bz + z_2 + z_3 + z_4 = 0,$$

$$-x_1 - y_1 = -3,$$

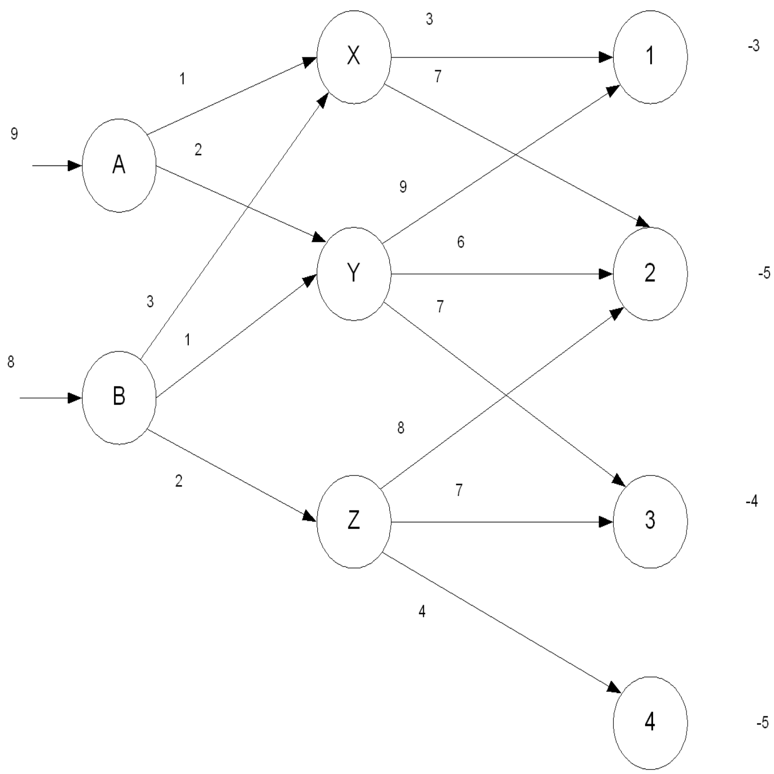

Figure 6.87: A transshipment problem.

$$
\begin{aligned}
&-x_2 - y_2 - z_2 = -5 \\
&-y_3 - z_3 = -4, \\
&-z_4 = -5.
\end{aligned}
$$

The "A" matrix is

		A	x	B	B	B	x	x	y	y	y	z	z	z
		x	y	x	y	z	1	2	1	2	3	2	3	4
		1	2	3	1	2	5	7	9	6	7	8	7	4
min	1													
9	2	1	1											
8	3			1	1	1								
0	4	-1		-1			1	1			$\cdots$			
0	5		-1		-1						$\cdots$			
0	6					-1					$\cdots$			
3	7						-1				$\cdots$			
-5	8							-1		$\vdots$				
-4	9									$\vdots$				
-5	10									$\vdots$				

The answer is $Ax = 8, Ay = 1, By = 3, Bz = 5, z_1 = 3, x_2 = 5, y_3 = 4, z_4 = 5$.

To solve the transshipment problem, we can use any of the following methods.

1. LP — but it is inefficient.
2. The transportation simplex method.
3. The network simplex method.

The network simplex method can solve may network LP problems. It solves the MCNFP (min cut / max flow problem). The MCNFP method can solve

1. Assignment problems.
2. Shortest route problems.
3. Maximum flow problems.
4. Transportation problems.
5. Transshipment problems.

The network simplex algorithm is just the transportation simplex with upper and lower bounds allowed on the arcs as well as the costs. In the assignment problem, you have n jobs and m workers. Worker $i, i = 1, 2, ..., m$ can do job j at a cost of c_{ij}. How can you best assign the workers to the jobs?

- LP formulation. This is similar to the traveling salesman problem without the constraints. There are no single cycles. Let
$$x_{ij} = \begin{cases} 1, & \text{if person } i \text{ does job } j. \\ 0, & \text{otherwise.} \end{cases}$$
Minimize
$$z = \sum_i \sum_j c_{ij} x_{ij},$$
subject to
$$\sum x_{ij} = 1, \forall i \text{ (person)},$$
$$\sum x_{ij} = 1, \forall j \text{ (job)},$$
$$x_{ij} = 0, 1.$$
- Network formulation. See Figure 6.88.

To solve the assignment problem, use the Hungarian method (must first set up dummy jobs or persons).

1. Subtract the row minimum from each row and the column minimum from each column.
2. Check to see if you can cover the resulting zeros by exactly n lines.
3. If not, subtract the smallest uncovered value from all other un-crossed, and add it to every other at the intersection of two crossed lines.
4. Now try to center the zeros with exactly n lines. If yes, done; the zeros represent the optimal solution x_{ij}. If not, return to Step (3).

So,

$$\begin{bmatrix} 1 & 2 & 3 \\ 1 & 4 & 3 \\ 1 & 2 & 5 \end{bmatrix} \to \begin{bmatrix} 0 & 1 & 2 \\ 0 & 3 & 2 \\ 0 & 1 & 4 \end{bmatrix} \to \begin{bmatrix} 0 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

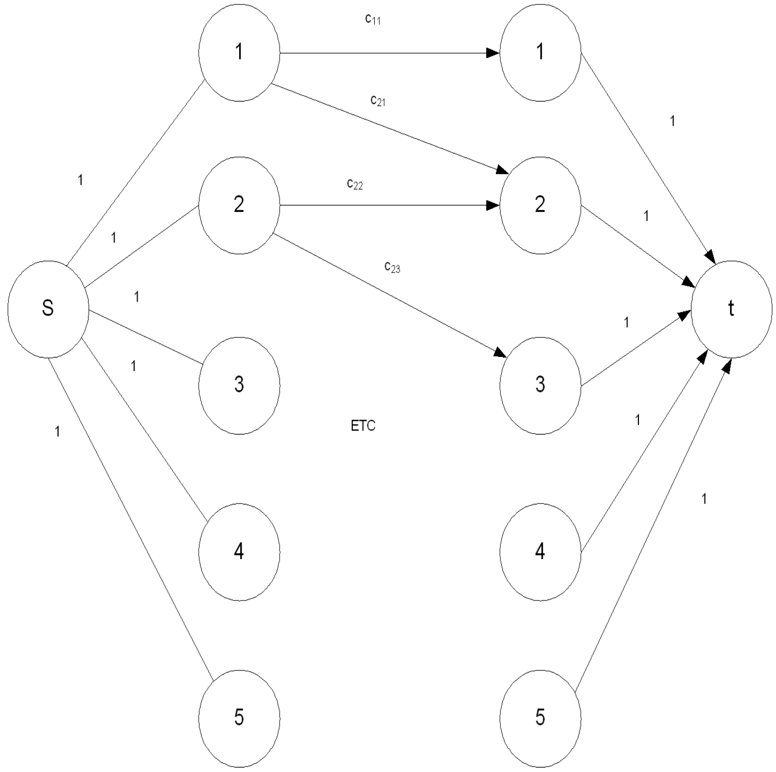

Figure 6.88: A network formulation of the assignment problem.

6.14 Network Location Problems

Locating facilities (i.e. a school, airport, etc) in such a way as it is convent for as many people along the network as possible. For example, we should be concerned with selecting the best location in a specified region for a service facility such as a shopping center, warehouse, etc. The nodes are the cities, and have demands associated with them. The math structure of a location problem depends on the region available for the location and on how we judge the quality of a location. Consequently, there are many different kinds of location problems. Should the facility be on the arc, node?

Example: A distribution system design. Suppose a firm did not own any warehouses. Then goods would be shipped directly from the plants to the retail stores. Warehouses placed close to the markets (sets of retail stores) can provide quick and efficient delivery to retail stores while still allowing factories to be near the suppliers. See Figure 6.89.

Warehouses must be located on a road network since trucks are commonly the choice of transport vehicles. The warehouses would be located either at the intersections (nodes) or along the roads (arcs) of the network. The typical objective is to minimize the total cost of shipping goods for both 1) from the factory to the warehouse and 2) from the warehouse to the retail stores.

Example: Bank account and lock box location. Consider the location of a post office box where VISA collects its payments. The number of days required to clear a check drawn on a bank in one city depends on the city in which the check is cashed. This time is called float and the payer will continue to earn interest on the funds until the check clears. For large corporations, the difference of even a few days can have significant monetary affects. Thus, to maximize its available funds, a company may decide to maintain accounts in several strategically located banks. It would then pay bills to clients in one city from a bank in some other city that had the largest clearing time (or float).

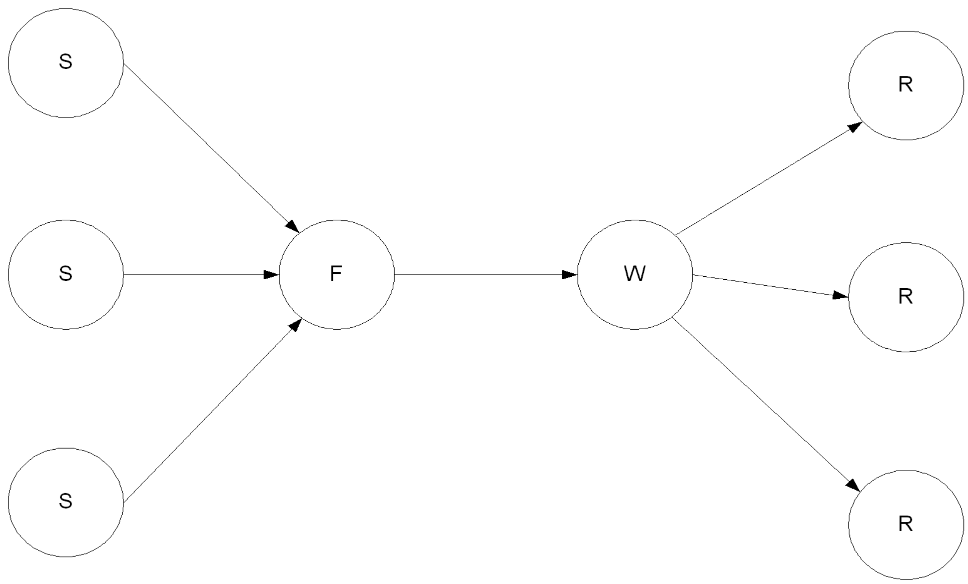

Figure 6.89: Warehouse example.

Example: The lock box example is opposite, but a related problem. The locations are decided on quickest clearance times. With regards to accounts receivable, corporations want to collect funds due to them as early as possible. This can be done by locating the check collection centers or lock boxes at strategic locations so that the float is minimized. If the cities are represented as nodes and the edges correspond to the information limits (postal times, etc) then both of these problems can be represented as location problems on a graph. We seek to locate the bank accounts or lock boxes at the vertices of the graph to optimize the appropriate objective.

Both of the above problems in the examples have a trade off because of the number of locations, and the maximum and minimum floats.

Example: Emergency facility location. Consider the problem of locating emergency facilities such as hospitals, fire stations, civil defense, or accident rescue. Except for helicopters, emergency vehicles must travel along a road network and the facility may be located either at on intersection or along some road segment. The usual objective is to place (locate) the facility so that the maximum response time to any point of demand is minimized.

Other examples of location problems include:

- Switching centers in communication networks.
- Computer facilities.
- Bus stops.
- Mail boxes, post offices, etc.
- Shopping centers, court houses, jails.

- Military supply points.

6.14.1 Classifying Location Problems

Some of the characteristics of location problems include:

1. Location of a facility is usually on a vertex. For example, a fire station could be an arc but an interstate highway exit will be at a node.
2. Location of demands are vertices and can be anywhere on the network. For example, houses are on roads; but in the lock box example, demands came from cities (nodes).
3. The objective function is usually to minimize the total cost for all demand points or to minimize the maximum cost.

Each *combination* of the 3 problem characteristics above results in a different problem, each with a unique name. We require more terminology for defining these problems.

1. A *center* is any vertex whose furthest vertex is as close as possible, In this case, both the facility and demands occur only at nodes.
2. A *general center* of a graph is any vertex whose furthest point in the graph is as close as possible. While the facility will be located at a node, demand points lie along edges as well as nodes.
3. An *absolute center* of the graph is any point whose furthest vertex is a close as possible. In this case, the facility is located anywhere on the network, but demands occur only at vertices.
4. A *general absolute center* of a graph is any point whose furthest point is as close as possible. Here, both facilties and demands are located anywhere on the graph.

In addition, we can define the following terms.

Median	Center
General Median	General Center
Absolute Median	Absolute Center
General Absolute Median	General Absolute Center

The *center* minimizes the maximum distance whereas the *medians* minimize the sum of the distances from the facility to all other demand points. See Figure 6.90.

Here are some examples:

1. A county has decided to build a new fire station which must serve all 6 townships in the county. The fire station is to be located somewhere along one of the highways in the county so as to minimize the distance to the township furthest from the fire station. See Figure 6.91. All the lengths are 1. Where is the absolute center? Eyeball it! For the problem set, eyeball it and argue why that is your best guess.

2. Now suppose the same county must locate a post office so the total distance is minimized. The absolute Median is the same as the absolute center. But there are multiple answers. See Figure 6.91. Anywhere along (2, 5) is optimal with a total distance of 7.

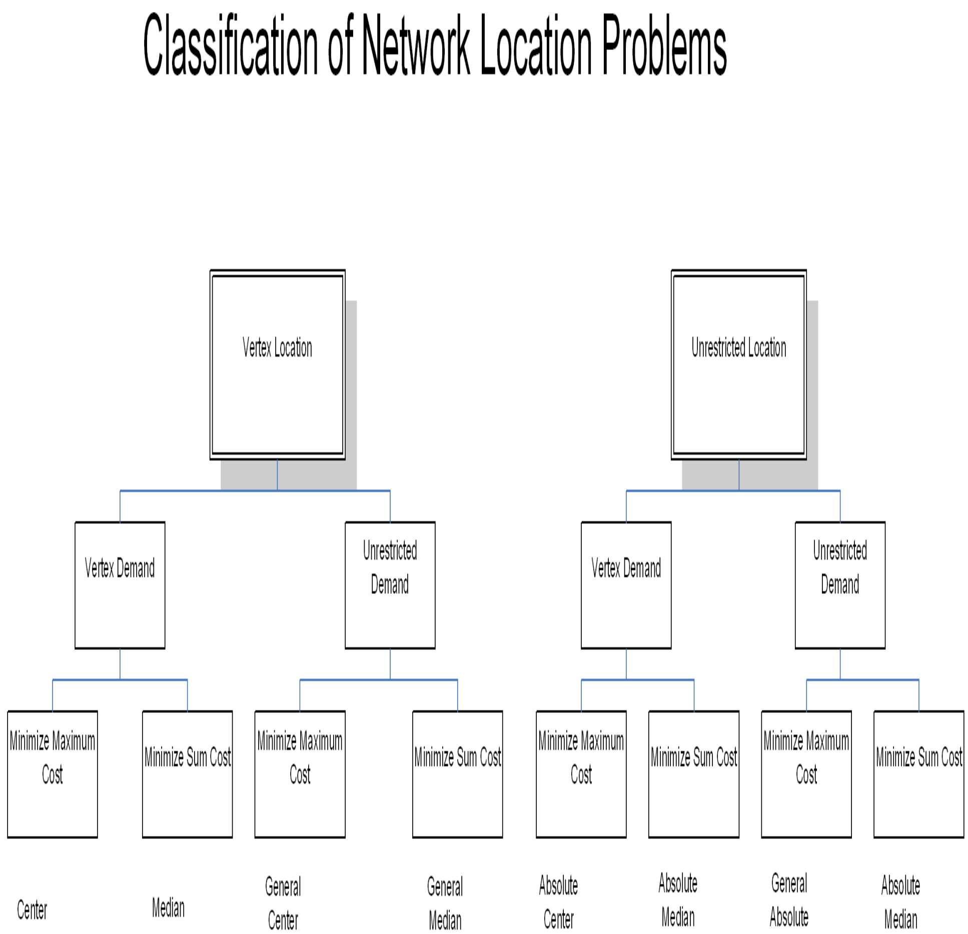

Figure 6.90: Classification of network location problems.

3. Now suppose that the same count must locate a station for how trucks rescue motorists who have become stranded somewhere on the county's highways. Suppose also that the potential location is judged according to the maximum distance a tow truck must travel to rescue a motorist. This is an absolute center. The problem is more complex. You must consider the maximum distance to all points on all arcs. All points and all arcs must be considered instead of just the maximum distance to a vertex. Also, the arcs could have *weights* representing the traffic intensity on each segment of the highway.

4. In this case, the county must select a location for a telephone switching station somewhere along a highway or in a town. The switching station stations must be located so as to minimize the total length of all telephone lines that must be laid. To complicate matters, the township has varying population sizes and require anywhere between one and five lines from themselves to the switching station. Note that this problem is a *weighted absolute median* problem. It is similar to problem (2), except that the nodes are weighted.

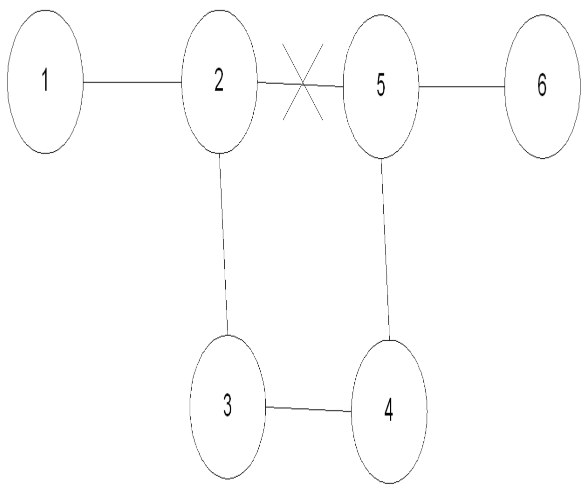

Figure 6.91: Fire station example where all arc lengths are 1.

Many variants of these problems have been studied. For instance, the objective is the maximize rather than minimize the distance to the facility.

6.14.2 Solutions to the Center Problems

Recall that a center is any vertex x with the property that the most distant vertex from x is as close as possible. To solve the center problem, we need the matrix D of shortest distances (found by Dijkstra's algorithm and others).

Example: Consider the graph in Figure 6.92. The corresponding D matrix is

$$D = \left[\begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & 2 & 3 & 3 \\ 2 & 4 & 0 & 2 & 1 \\ 3 & 6 & 2 & 0 & 3 \\ 4 & 3 & 5 & 4 & 0 \end{array}\right]$$

The matrix is not symmetric because of the directed arcs in the graph. The center is that vertex with the shortest maximum distance. So, a simple solution is to look across the columns of D and see that row 1

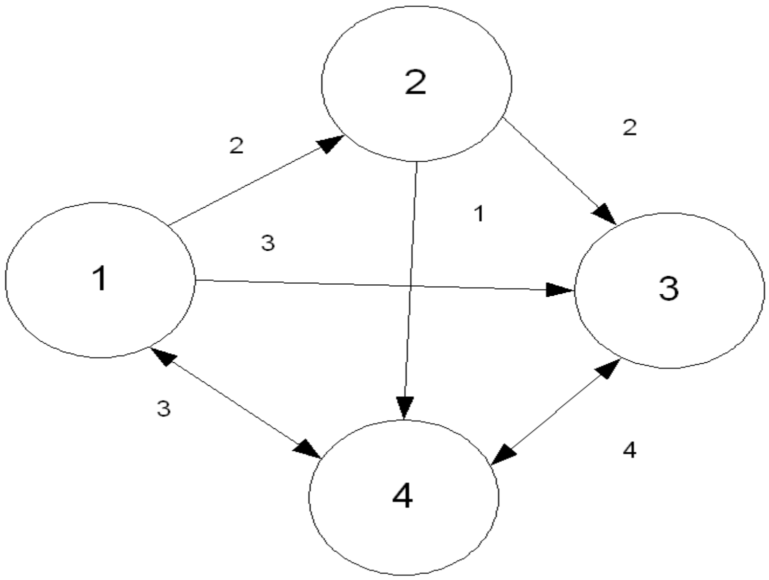

Figure 6.92: Center location example.

has the minimum maximum distance. So, put the facility at the center of node 1.

This problem was easy because only vertices were considered. The general center problem has the facility location on a vertex but the demands along the arcs. We now need a matrix D' (obtained from D) representing the shortest distance from vertex j to a point on the arc (r, s). For some point on (r, s), this distance takes on its maximum value denoted by $d'(j, (r, s))$ and is called a *vertex-arc distance.* This vertex-arc distance depends on whether (r, s) is directed or undirected.

For undirected arcs:

$$d'(j(r,s)) = \frac{d(j,r) + d(j,s) + a(r,s)}{2}.$$

See the top part of Figure 6.93.

For directed arcs, $d'(j(r, s)) = d(j, r) + a(r, s)$. See the lower part of Figure 6.93. You need to do this with even one directed arc (r, s) because we want to go to the points along (r, s) which cannot get to from s!

This is an actual SAT question. See Figure 6.94. Given two lengths 5" x 8", (A, B) and (A, C) what distance (C, B) is needed in order to form a triangle? $3 < (C, B) < 13$ because $(A, C) - (A, B) < (C, B) < (A, B) + (A, C) \rightarrow 8 - 5 < (C, B) < 8 + 5$. The triangle inequality is $A + B > C$. What is the maximum distance from j to a point on (r, s)? 7. See Figure 6.95. $\max 7 = d(j, r) + d(r, s)$. Now with undirected arcs, what is the maximum distance? $6 = \frac{3+5+4}{2}$. See Figure 6.96. Note: In using the formulas, we must assume that the triangle inequalities $a + b > c$ works! For example, consider Figure 6.97. This could never be a real triangle, and it does not satisfy the triangle inequality; can't get the maximum distance to any point on this arc because the formula gives $\frac{2+20+72}{2} = 47$ which is not even on the arc desired!

Recall the example in Figure 6.100 on page 432. We labeled the arcs

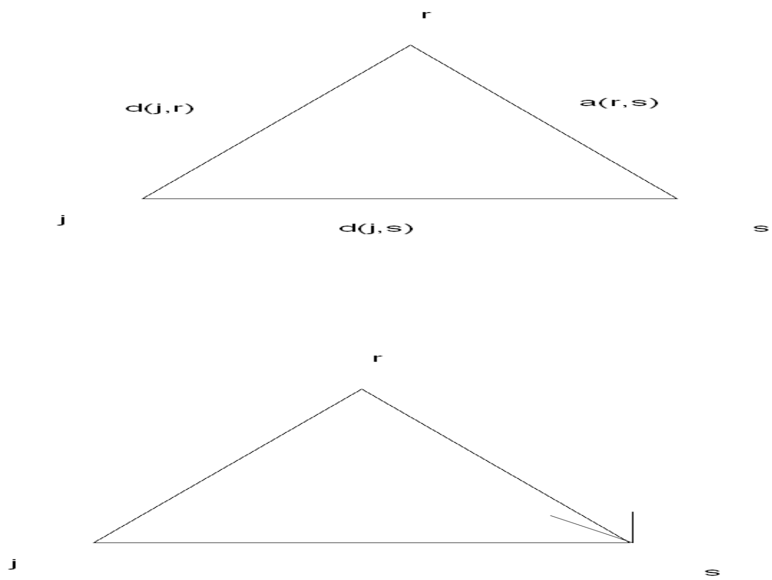

Figure 6.93: Vertex-Arc distance.

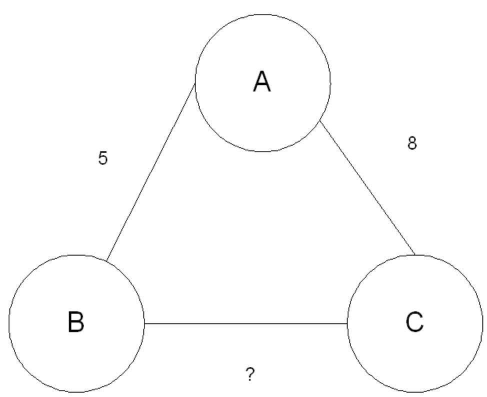

Figure 6.94: Actual SAT question.

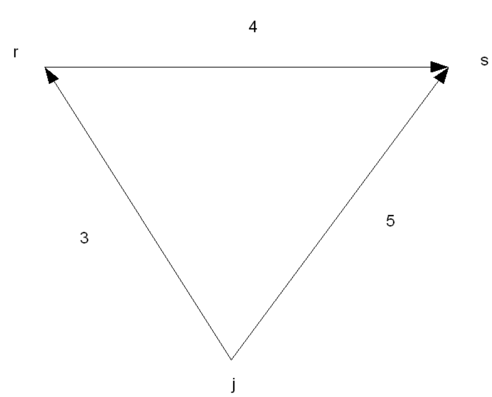

Figure 6.95: Actual SAT question with directed arcs.

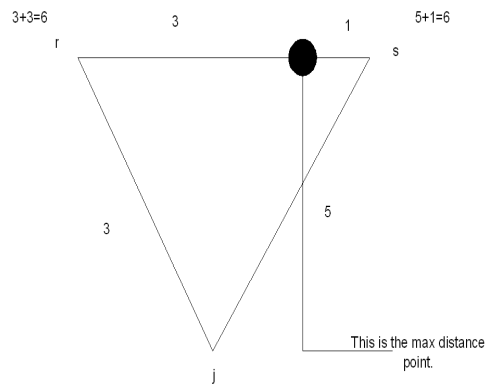

Figure 6.96: Actual SAT question with un-directed arcs.

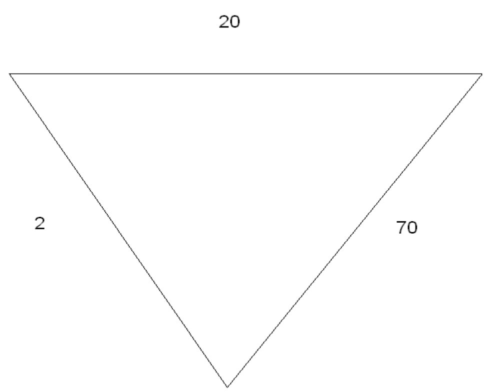

Figure 6.97: Example of a triangle that can never be real.

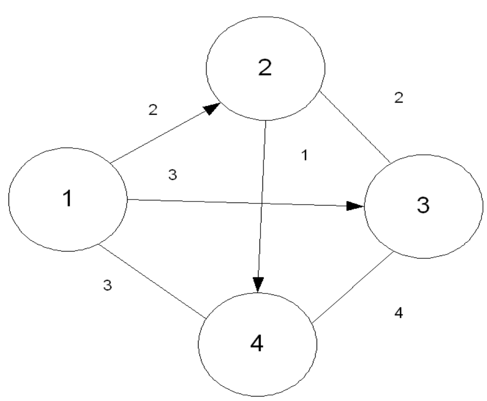

Figure 6.98: A graph from a previous example.

Arc	Number
$(1,2)$	1
$(1,3)$	2
$(1,4)$	3
$(2,4)$	4
$(2,3)$	5
$(3,4)$	6

This is used with D'. Recall that

$$D = \left[\begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & 2 & 3 & 3 \\ 2 & 4 & 0 & 2 & 1 \\ 3 & 6 & 2 & 0 & 3 \\ 4 & 3 & 5 & 4 & 0 \end{array}\right]$$

$$d'(j(r,s)) = \begin{cases} \frac{d(j,r)+d(j,s)+a(r,s)}{2}, & \text{For undirected arcs.} \\ d(j,r)+a(r,s), & \text{For directed arcs.} \end{cases}$$

For example, $d'(1,(3,4)) = \frac{1}{2}[d(1,3)+d(1,4)+a(3,4)] = \frac{1}{2}[3+3+4] = 5$. $d'(1,(2,4)) = d(1,2)+a(2,4) = 2+1 = 3$, etc. And so, we get D' which is the vertex-arc distance matrix.

$$D' = \left[\begin{array}{c|cccccc} & 1 & 2 & 3 & 4 & 5 & 6 \\ \hline 1 & 2 & 3 & 3 & 3 & 3.5 & 5 \\ 2 & 6 & 7 & 4 & 1 & 2 & 3.5 \\ 3 & 8 & 9 & 6 & 3 & 2 & 3.5 \\ 4 & 5 & 6 & 3 & 6 & 5.5 & 4 \end{array}\right]$$

Because of the triangle inequality...it limits this algorithm. Granted that Figure 6.99 is not allowed in general geometry, but in the real world, the arcs are not necessarily straight time and since we take a real world situation and make it look geometric. Figure 6.99 becomes Figure 6.97. The MVA(i), the maximum vertex arc distance from node i are as follows: MVA(1) = 5, MVA(3) = 9, MVA(2) = 7, MVA(4) = 6. Node 1 is the best choice. It is the "closest" to all points over all other node choices. So, node (vertex) 1 is a *general center* of the graph. The furthest point from 1 is 5 units and lies on (3,4).

Homework Notes: The absolute center and general center can be at either end. Eyeball the answers in the problem sets. Remember, no *interior point* of a directed arc can be an absolute or general absolute center! Because, you can not go both ways from it!

With our example, see Figure 6.100 for the eyeball absolute centers. Note that we can eliminate arcs (1,2), (2,4) and (1,3) because they are directed arcs. So, we must consider nodes 1, 2, 3, and 4; and arcs (2,3), (1,4), and (3,4). Vertex 1 is the absolute center with a maximum distance of 3 to all other vertices.

6.14.3 Median Problems

Recall that a *median* is any vertex x with the smallest possible total distance from x to all other vertices. Recall that when finding the center, we took the maximum over the rows of the shortest distance matrix D. To find the median of the graph, we merely sum over each row and take the minimum value. So, the median problem looks more at clusters rather than outliers. Thus, for our example, recall D

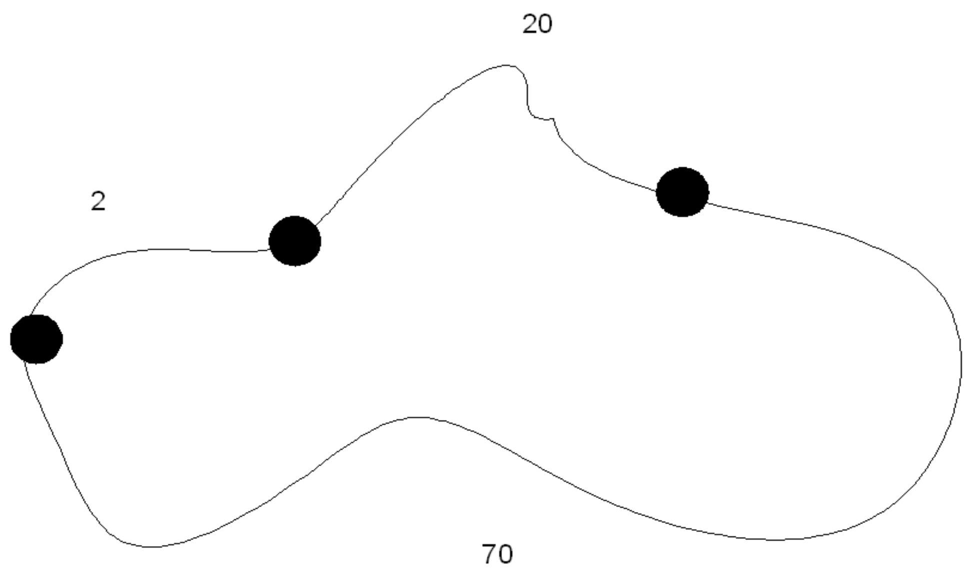

Figure 6.99: Center location example with un-directed arcs.

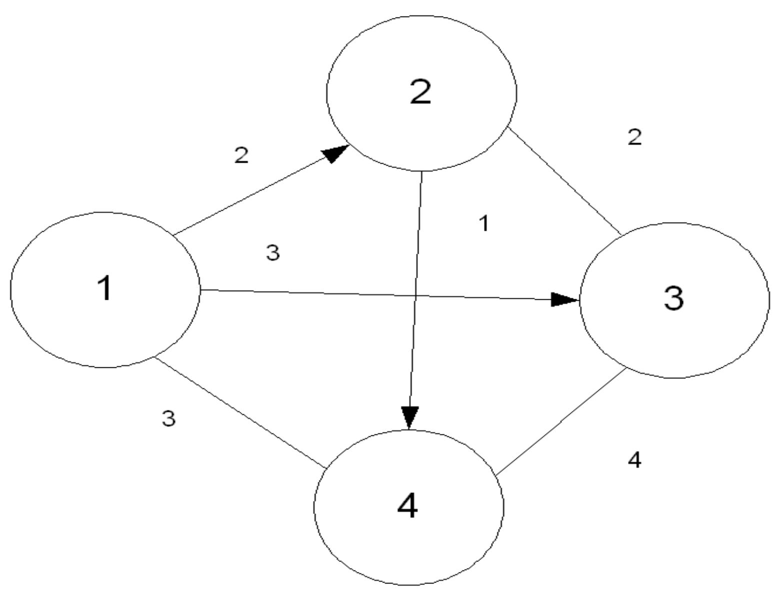

Figure 6.100: Eyeball the absolute centers.

$$D = \left[\begin{array}{c|cccc|l} & 1 & 2 & 3 & 4 & \text{Sum} \\ \hline 1 & 0 & 2 & 3 & 3 & 8 \\ 2 & 4 & 0 & 2 & 1 & 7(Best) \\ 3 & 6 & 2 & 0 & 3 & 11 \\ 4 & 3 & 5 & 4 & 0 & 12 \end{array}\right]$$

So, choose vertex 2 as the median.

General Median

The general median is any vertex x with the smallest total distance to any arc where the distance from a vertex to an arc is taken to be the maximum distance from the vertex to the points on the arc. Thus, to find the general matrix, we need only to sum across the rows of the D' matrix and choose the minimum.

$$D' = \left[\begin{array}{c|cccccc|l} & 1 & 2 & 3 & 4 & 5 & 6 & \text{Sum} \\ \hline 1 & 2 & 3 & 3 & 3 & 3.5 & 5 & 19.5(Best) \\ 2 & 6 & 7 & 4 & 1 & 2 & 3.5 & 23.5 \\ 3 & 8 & 9 & 6 & 3 & 2 & 3.5 & 31.5 \\ 4 & 5 & 6 & 3 & 6 & 5.5 & 4 & 29.5 \end{array}\right]$$

Thus, the general median is vertex 1. Again, no directed arc's interior point will be an absolute median or general absolute median.

Theorem: There is always a vertex that is an absolute median (i.e. a vertex that is at least as good as any point on an arc).

So, there may be ties with points on the arcs, but you know you have an absolute median by using the original median problem for an answer. For the general absolute medians, the solution procedures involve searching and an iterative procedure which we will not cover.

Extensions

1. Weighted Locations. For many practical problems, a vertex has a different importance or weight in the problem. Weights may correspond to population demand, supply, cost, etc. Arcs may have weights as well; for example if the arcs represent highway segments that must be served from a central emergency station, each segment should be weighted according to the amount of traffic it carries.

2. Multi-Centers versus Multi-medians. These are very difficult, and we will not cover them in this class. The general set-up is as follow for weights on a graph.

$$D = \left[\begin{array}{ccccc} & w_1 & w_2 & w_3 & w_4 \\ \hline 1 & & & & \\ 2 & & & & \\ 3 & & & & \\ 4 & & & & \end{array}\right]$$

Only apply the weights once in D. The weights are on the nodes. Multiply the columns by the weights and solve a usual.

$$D' = \begin{array}{c|cccccc} & w_1 & w_2 & w_3 & w_4 & w_5 & w_6 \\ \hline 1 & & & & & & \\ 2 & & & & & & \\ 3 & & & & & & \\ 4 & & & & & & \\ & & & & & & \end{array}$$

6.15 Euler Networks and Postman Problems

The Chinese postman problem (and related arc routing problem) is as follow: consider a network. The problem is to find a minimum distance path which traverses all the arcs at least once (called CPP). Edges can be directed, undirected or both.

Example: Consider street sweepers, snow plows, interstate lawn mowers, police patrol cars, automated guided vehicles, etc.

Special cases of the CPP include np-complete and np-hard (we will not cover these).

1. Capacitated CPP (CCPP). Each arc has possible demand and the vehicles have a finite capacity. Example: School buses, road salting trucks, etc. The route is constrained by capacity and may not be able to cover all arcs.
2. Capacitated Arc Routing Problem (CARP). Not all of the arcs have demands. We do not want to eliminate all no-demand arcs. Example: County responsible for patrolling county roads, but we can only travel on state roads. Then, only a subset of arcs will be traversed.

6.15.1 Euler Tours

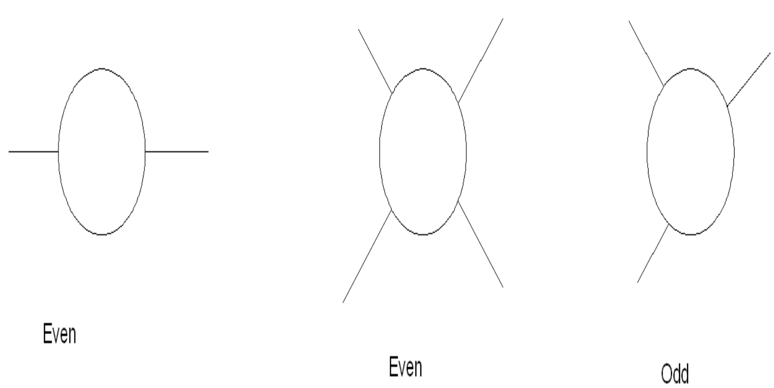

Figure 6.101: Examples of even and odd degree nodes.

Recall the Kongsberg bridge problem in Figure 6.2 on page 319. He proved that you can not cross every arc exactly once and make it home. But if you can do this, then you have a Euler tour. Any cycle in a graph that crosses an edge exactly once is called an a Euler tour. Any graph that possesses a Euler tour is called a *Euler graph.* If you can find a Euler tour, the CPP is solved because crossing an arc only once is the minimum path. The exact order does not matter. *Dead heading* is when you cross an arc twice because you must. So, if you have a Euler tour, the number of times a postman arrives at a vertex must equal the number of times he leaves. This is similar to Markov chains. If the postman does not repeat any edges incident to a vertex, then this vertex must have an even number of edges incident to it, or an *even degree.* See Figure 6.101.

Theorem: An undirected graph is Euler iff all vertices have an even degree.

Example: See the upper part of Figure 6.102. There are four different, equally valid Euler tours. All of them have the same distance length of 22.

Example: See the lower part of Figure 6.102. This is a graph with no Euler tour. The amount of Dead heading is 5 — for arc (2,4) which must be traversed twice. The idea behind graphs with out a Euler tour is to search for ways to minimize Dead heading.

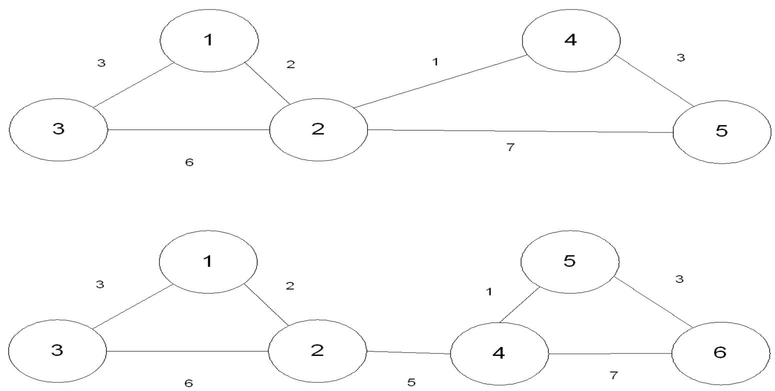

Figure 6.102: Postman examples with even and odd degree nodes.

6.15.2 Constructing Euler Tours

Suppose we have a Euler graph (or any graph) $G = (x, E_1)$. If a graph possesses a Euler tour then we have Dead heading. Note that the sum of all of the lengths is constant. The CPP can be interpreted as minimizing the amount of Dead heading.

The steps of construction of the Euler graph are as follow.

1. Begin at any vertex and construct a cycle C. Traverse any edge (s, x) incident to s and mark this edge "used." Next, traverse any unused edge incident to x. Repeat until you return to s. We must be able to return to s since G is a Euler graph. If we enter node i, we can leave it, and we can return to node s.

2. If your cycle C contains all edges of G, then stop. If not, then a subgraph G' in which all edges of C are removed must be Euler since the vertex of C must have an even number of edges. Since G is connected, there must be at least one vertex V in common with C. We know we can start a new cycle (ignoring arcs used in C) at V and it will be connected to C by only looking at the left-over arcs in the subgraph.

3. Splice together the cycles C and C' and call it C. Return to step 2 and repeat until all of the arcs are used.

Example: See Figure 6.103. $C = \{a, f, h, i\}, V = 2$ and 5. Use node 2. $C' = \{e, g, d, c, b\}, C + C + C' = \{a, b, c, d, e, f, g, h, i\}$ all of G. The cycle is $\{a, b, c, d, g, e, f, h, i\}$.

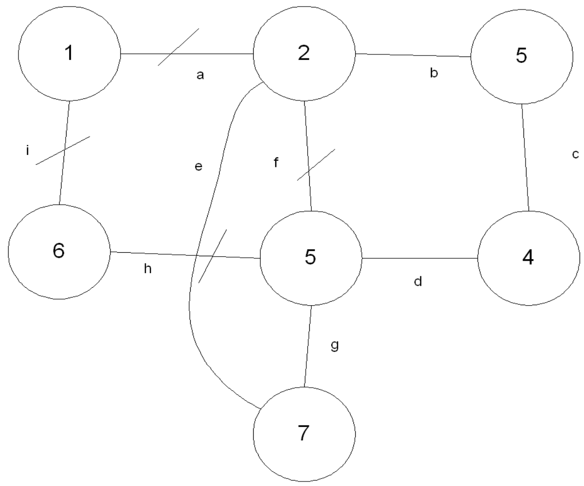

Figure 6.103: The example of constructing a cycle and splicing.

6.15.3 The Chinese Postman Problem for Undirected Graphs

If G is not a Euler graph, then minimize Dead heading. Let $a(i, j)$ be the length of edge (i, j) in G. In any postman route, the number of times the postman enters a vertex equals the number of times the postman leaves that vertex. Therefore, if vertex x does not have an even degree, then at least one edge incident to x must be repeated by the postman. Let $f(i, j) + 1$ denote the number of times that (i, j) is traversed by the postman so that $f(i, j)$ is the number of times (i, j) is repeated. Of course $f(i, j)$ is a non-negative integer. Note that $f(i, j)$ contains no information about the direction that (i, j) was traveled across. Construct a new graph $G^* = (x, E^*)$ that contains $f(i, j) + 1$ copies of each edge (i, j) in graph G. Clearly, a Euler tour of graph G^* corresponds to a postman route in graph G. The postman wishes to select values for the $f(i, j)$ variables so that:

1. Graph G^* is an even graph.
2. $\sum a(i, j)f(i, j)$ is minimized which is the total length of a repeated edge.

If the vertex x is an odd degree vertex in G, then an odd number of edges incident to x must be repeated by the postman so that in graph G^*, vertex x has an even degree. Similarly, if x has an even degree vertex in G, an even number of edges (may be zero) must be repeated. See Figure 6.2 on page 319 and Figure 6.105.

With n odd degree nodes, you will have $\frac{n}{2}$ arcs to fix it (or more), but you may have a choice. Figure 6.104 shows how to fix the Kongsberg bridge problem. But, which real arcs belong on this artificial one (dashed line arc)? Therefore, the postman must decide:

1. Which odd-degree vertices will be joined by a path of repeated edges. See Figure 6.106.
2. The precise composition of the path.

One solution method is to arbitrarily join the odd-degree vertices by paths of repeated edges and use this theorem:

Theorem: A feasible solution to the postman problem is optimal iff (i) no more than one duplicated edge is added to any original edge and (ii) the length of the added edges in any cycle does not exceed $\frac{1}{2}$ the length of the cycle.

Lemma: If two feasible solutions satisfy (i) and (ii), then the lengths of their added edges are equal.

Lemma: An optimal solution always exists.

One problem arises when the number of cycles that must be checked in (ii) grows exponentially in the size of the graph. Thus, the algorithm cannot be performed in polynomial time. The method that we will use is the polynomial time algorithm which uses the shortest route algorithm. We can determine a shortest path because at each pair of odd degree vertices, they are in G. See Figure 6.107. Vertices 1, 3, 4, and 6 are odd degrees. Find the shortest path for all pairs of these vertices. Note that this is a symmetric matrix, and only the lower values have been filled in.

$$\left[\begin{array}{c|cccccc} & 1 & 2 & 3 & 4 & 5 & 6 \\ \hline 1 & 0 & & & & & \\ 2 & 1 & 0 & & & & \\ 3 & 4 & 5 & 0 & & & \\ 4 & 2 & 3 & 2 & 0 & & \\ 5 & 4 & 5 & 7 & 6 & 0 & \\ 6 & 3 & 2 & 4 & 3 & 3 & 0 \end{array}\right]$$

Now, as a subproblem, ignore all the even degree nodes. So we look only at nodes 1, 3, 4, and 6. Form the sub-graph in Figure 6.108. There are three ways to fix this graph. Since this is a small example, we will enumerate all the different ways. (1, 4) and (3, 6) have a cost of 6; (1, 3), and (4, 6) have a cost of 7; (1, 6) and (3, 4) have a cost of 5 (this path is best). The values for the arcs can be read from the shortest path matrix for larger, more complex problems.

For larger problems, use the *maximum weight matching algorithm.* Essentially, you create pairs of nodes in the best possible way (i.e match nodes). See Figure 6.109. The new graph G^* is a Euler graph. All the nodes have an even degree. An optimal route is 1-2-6-5-1-3-6-4-3-4-1-6-1.

6.15.4 The Postman Problem for Directed Graphs

For directed graphs, it is possible that no postman route exists. See Figure 6.110. Several algorithms exist for directed and mixed graphs.

Example: Vehicle Parking Problems. A number of customers with known delivery requirements and locations are the vehicles in a network. A fleet of trucks with limited capacity is available What customers should be assigned to different routes to minimize the total time or distance traveled? For example, we are routing a fleet of gasoline trucks to gasoline stations. Each station requires a fixed amount of gasoline to refill the tanks.

Assume that each vehicle has a fixed capacity W. Let $d(i)$ be the demand at vertex i and $a(i, j)$ be the cost or time associated with traveling from i to j. Assume also that all the vehicles are dispatched from a central depot, vertex O. An efficient heuristic algorithm (1963) is called the *savings approach.* Begin with an initial solution in which each customer is served *individually* from the depot. This is not optimal, but a feasible initial solution. Start with this solution and try to combine trips. Compute the savings incurred by combining routes. You must check the capacity as you combine the routes. Savings: $s(i, j) = a(0, i) + a(0, j) - a(i, j)$. See Figure 6.111. If the savings is greater than zero, then the routes are worth considering.

The steps to the savings algorithm are:

1. Compute the savings $s(i, j)$ for all pairs (i, j).

2. Choose the pair with the largest savings and check for feasibility (is less than or equal to W). If yes, the join; if no, then discard.

3. Continue as long as savings are possible. Stop when all possible savings have been considered.

This heuristic algorithm always gives a feasible solution, but the greedy approach can get you into trouble.

Example: Consider the following problem.

Customer	1	2	3	4	5	6	7
Demand	46	55	33	30	24	75	30

Note that the following matrix is symmetric. Again, only the lower part of the matrix has been filled in.

	0	1	2	3	4	5	6	7
0	–							
1	20	–						
2	57	51	–					
3	51	10	50	–				
4	50	55	20	50	–			
5	10	25	30	11	–			
6	15	30	10	60	60	20	–	
7	90	53	47	38	10	90	12	

The capacity is 80. We begin with 7 routes, 0-1-0, 0-2-0, ..., 0-7-0. Now compute the savings. For example, linking $s(1,2) = a(0,1) + a(0,2) - a(1,2) = 20 + 57 - 51 = 26$. Is the capacity ok? $d_1 + d_2 \le 80$? Since $46 + 55 > 80$, we can't do it. This is the savings matrix (ignoring capacity).

	1	2	3	4	5	6	7
1	–						
2	26	–					
3	61	58					
4	15	87	51	–			
5	5	37	50	10	–		
6	5	62	6	5	5	–	
7	57	100	103	130	10	93	–

Examine all possibilities — is the capacity ok? Choose the best first. Nodes 4 and 7 have a savings of 130 with a capacity of $30+30 = 60$. So, this one is ok. Continue with the rest of the matrix. We get the following routes: 0-4-7-0, 0-3-1-0, 0-2-5-0, 0-6-0. We are not guaranteeing these are optimal. The method is a greedy heuristic and easy to put on a computer.

6.16 References

1. Evans and Minieka, *Optimization Algorithms for Networks and Graphs (Chapters 8 and 10).*

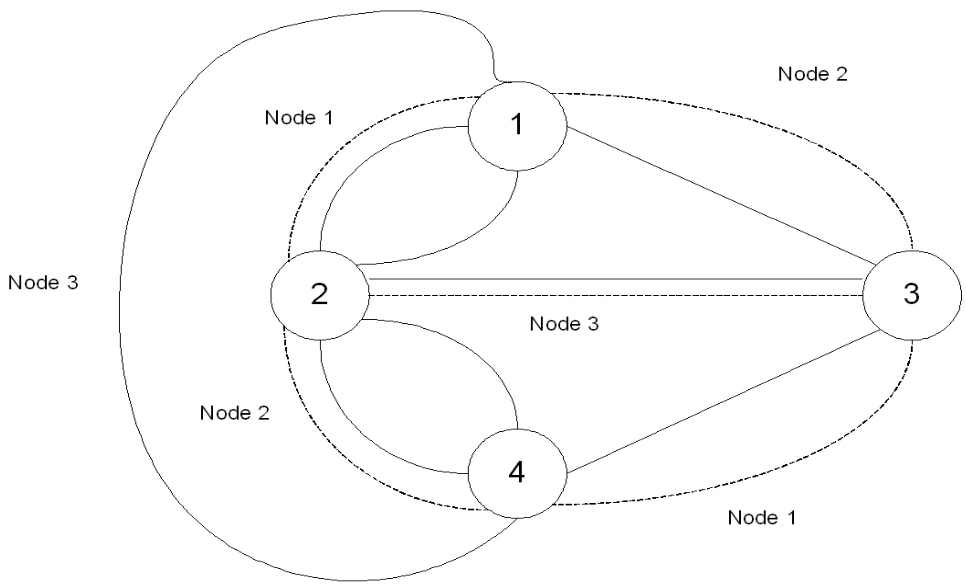

Figure 6.104: The Kongsburg Bridge with additional arcs.

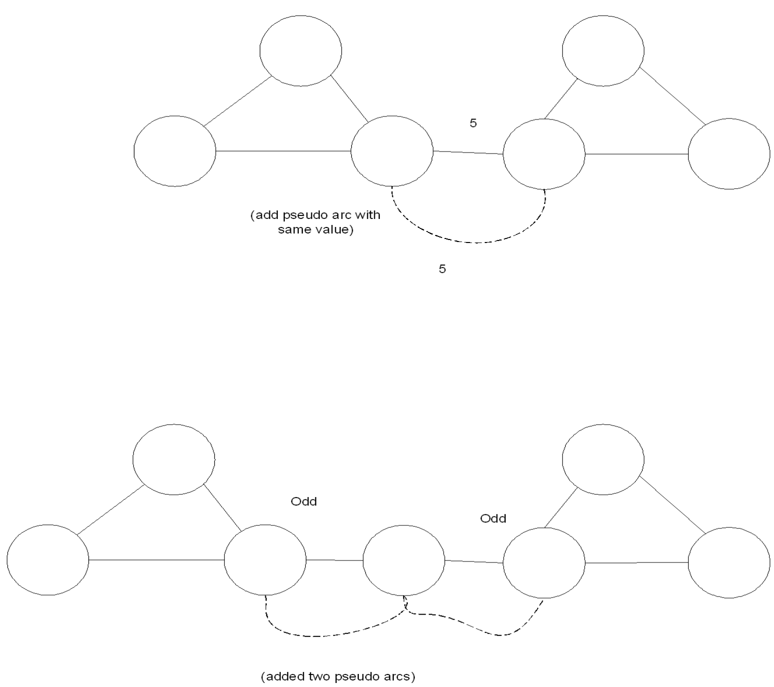

Figure 6.105: Examples of adding pseudo arcs to a graph.

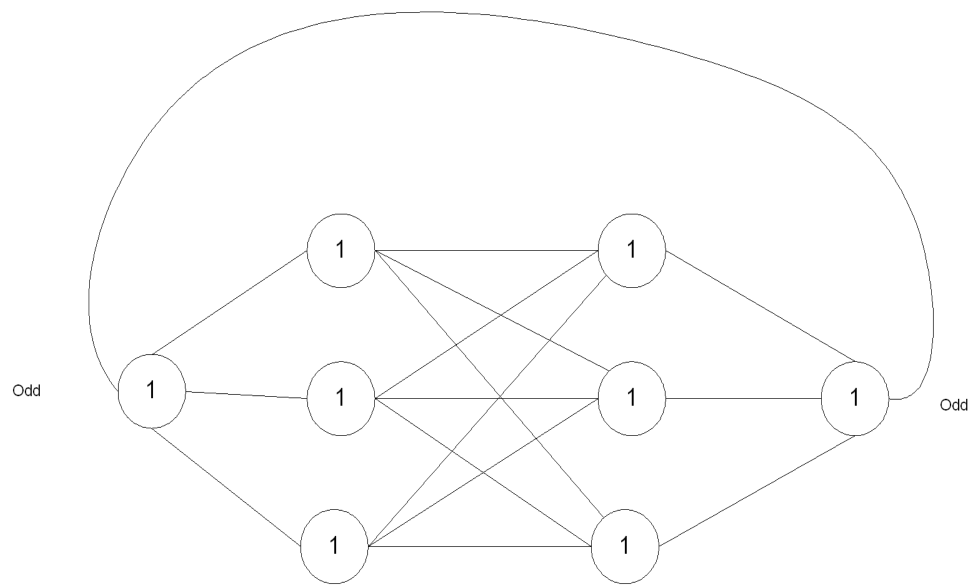

Figure 6.106: The Postman problem with odd degree arcs.

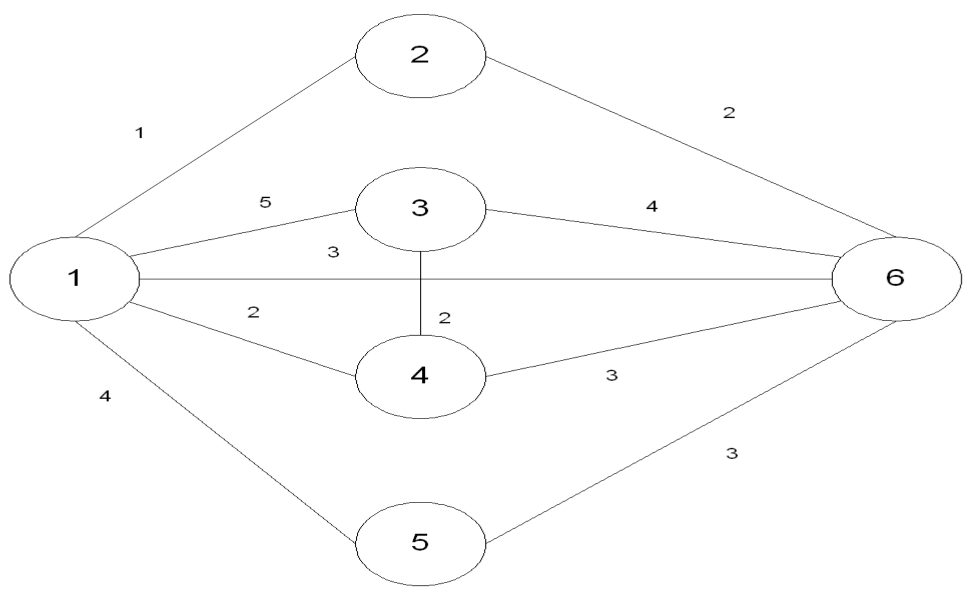

Figure 6.107: A graph with odd degree vertices.

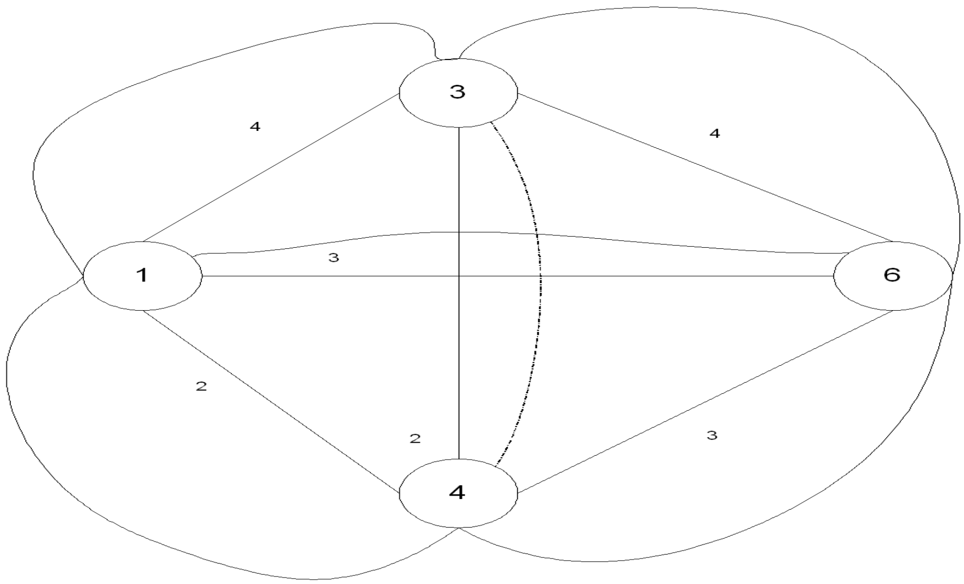

Figure 6.108: A subgraph for the graph with odd degree vertices.

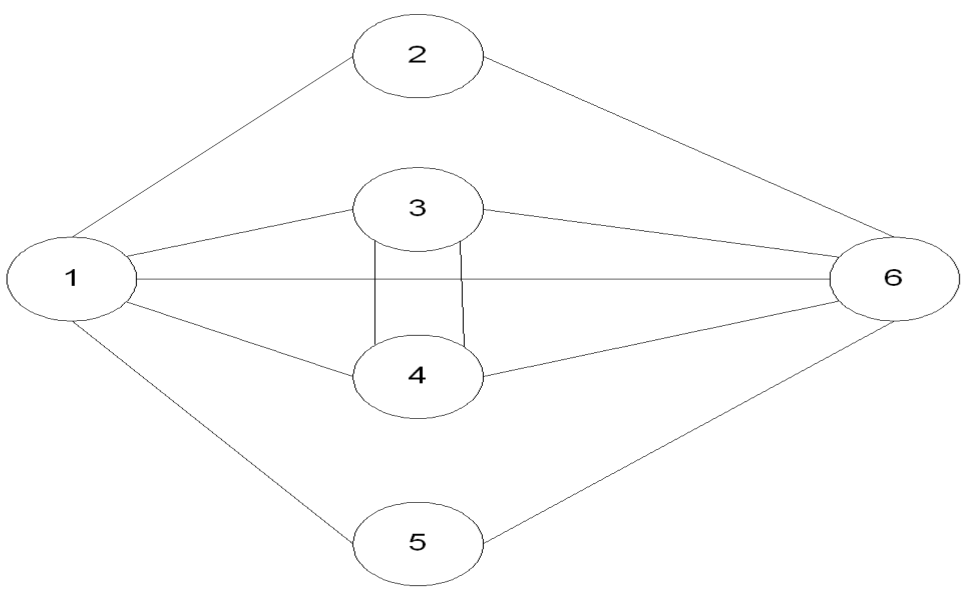

Figure 6.109: The new graph is now a Euler graph.

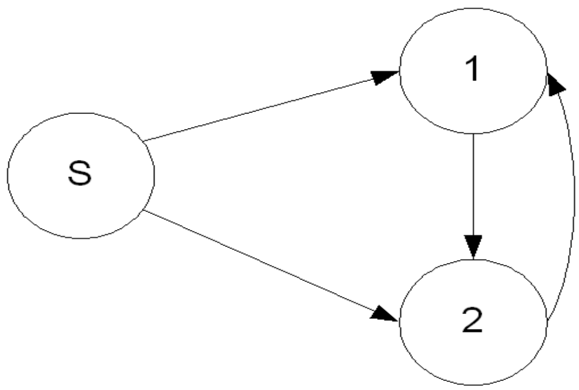

Figure 6.110: A directed graph with out a postman route.

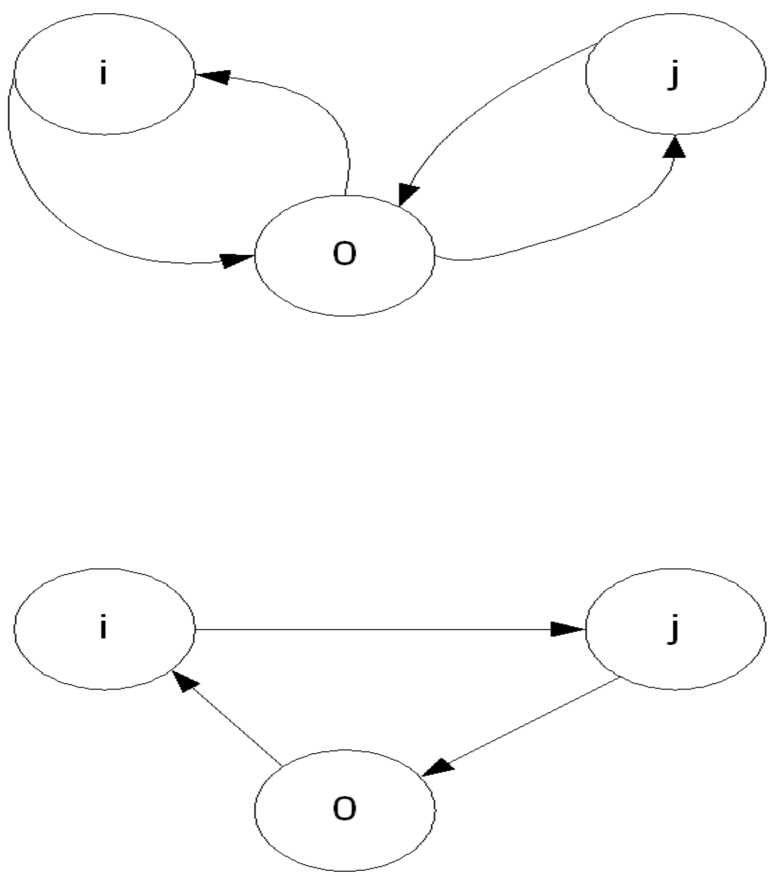

Figure 6.111: Calculating savings.

Chapter 7

Theory of Statistics

Old Dominion University

Dr. Ram Dahiya, Statistics 531, Spring 1996

Text used: Robert V. Hogg and Elliot A. Tanis, *Probability and Statistical Inference,* Prentice Hall, 1988

7.1 Estimating Parameters

7.1.1 Inference Based on Random Samples

Example: Does smoking cause lung cancer? Let p_1 be the proportion of people who die of lung cancer who smoke. Let p_2 be the proportion of people who die of lung cancer who do not smoke. Suppose $\frac{p_1}{p_2} = 20\%$. p_1 and p_2 are parameters of the population. Random samples must be taken to estimate p_1 and p_2.

Suppose we have a population and we select a subject. X is equal to an observation on the selected subject. Assume X has a pdf $f(X|\theta)$, and θ is an unknown parameter.

Example: $X \sim N(\theta_1, \theta_2)$; Let $X_1, X_2, ...X_n$ be a random sample. $\hat{\theta} = U(x_1, x_2, ..., x_n)$ is an estimator for θ. We want $\hat{\theta} - \theta$ to be the error in $\hat{\theta}$ for estimating θ. Specifically, $P(-a < \hat{\theta} - \theta < a)$ should be large for small values of a. When $E(\hat{\theta} - \theta) = B(\hat{\theta})$, it is called *the bias of* $\hat{\theta}$. We want $E(\hat{\theta} - \theta) = E(\hat{\theta}) - \theta = 0$, and we want $Var(\hat{\theta})$ to be as small as possible.

$$Var(\hat{\theta}) = E(\hat{\theta} - E(\hat{\theta}))^2 = E(\hat{\theta} - \theta)^2,$$

if $E(\hat{\theta}) = \theta$. In other words, the bias is zero. $\hat{\theta}$ is known as an *unbiased estimator* if $B(\hat{\theta}) = 0$, when $e(\hat{\theta}) = \theta$.

Example: Suppose there are n workers, $x_1, x_2, ..., x_n$. Let d be the location of the office. Minimize the total distance traveled by the workers.

$$\sum_{i=1}^{n} |x_i - d|$$

is the *median.* d should be the median. Minimize

$$K(d) = \sum_{i=1}^{n} (x_i - d)^2$$

if small distances do not matter.

$$\frac{dK(d)}{dd} = \sum_{i=1}^{n} -2(x_i - d) = 0. \qquad \sum_{i=1}^{n} \frac{x_i}{n} - \sum_{i=1}^{n} \frac{d}{n} = 0. \qquad \bar{x} - d = 0. \qquad d = \bar{x}.$$

Suppose $E(x) = \mu$ and $Var(x) = \sigma^2$. $x_1, x_2, ..., x_n$ is a random sample. Then

$$\bar{x} = \sum_{i=1}^{n} \frac{x_i}{n}.$$

$$E(\bar{x}) = \frac{1}{n}\sum_{i=1}^{n} E(x_i) = \frac{1}{n}\sum_{i=1}^{n} \mu = \frac{n\mu}{n} = \mu.$$

$\bar{x}$ is an unbiased estimator of μ. What about σ^2? The sample variance,

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2.$$

Fact: S^2 is an unbiased estimator of σ^2. Proof:

$$\sum_{i=1}^{n}(x_i - \bar{x})^2 = \sum_{i=1}^{n} x_i^2 - n\bar{x}^2.$$

$$E\left(\sum_{i=1}^{n}(x_i - \bar{x})^2\right) = E(x_i^2) - nE(\bar{x}^2).$$

Remember that $\sigma^2 = E(x^2) - \mu^2 = Var(x)$.

$$E(x^2) = \sigma^2 + \mu^2.$$

$$E(\bar{x}^2) = Var(\bar{x}) + [E(\bar{x})]^2 = \frac{\sigma^2}{n} + \mu^2.$$

So,

$$\sum_{i=1}^{n}(\sigma^2 + \mu^2) - n\left(\frac{\sigma^2}{n} + \mu^2\right) =$$

$$n\sigma^2 + n\mu^2 - \sigma^2 - n\mu^2 =$$

$$(n-1)\sigma^2.$$

$$E\left(\sum_{i=1}^{n}(x_i - \bar{x})^2\right) = (n-1)\sigma^2$$

$$E\left(\frac{\sum_{=1}^{n}(x_i - \bar{x})^2}{n-1}\right) = \sigma^2$$

$$E(S^2) = \sigma^2.$$

Suppose we know μ. An estimator of σ^2 is

$$\sigma^2 = E(x^2) - \mu^2 = \sum_{i=1}^{n} \frac{x_i^2}{n}$$

is an estimator of $E(x^2)$.

$$\sum_{i=1}^{n} \frac{x_i^2}{n} - \mu^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2.$$

We know that $E(S^{*2} = \sigma^2)$ and $E(S^2) = \sigma$. S^{*2} is a better estimator by showing it has a smaller variance than S^2. The Mean Square Error(MSE) of $\hat{\theta}$ is $E(\hat{\theta} - \theta)$. $\hat{\theta}$ is an estimator of θ. $\hat{\theta}$ is the minimum MSE estimator of θ if

$$E(\hat{\theta} - \theta)^2 \leq E(\tilde{\theta} - \theta)^2,$$

for any other estimator $\tilde{\theta}$. Suppose that $\hat{\theta}$ is unbiased for $\theta(E(\hat{\theta}) = \theta)$. Then, $MSE(\hat{\theta}) = Var(\hat{\theta})$. If dealing with unbiased estimators, then one only needs to look at the variance. If the estimator is bias, then

$$MSE(\hat{\theta}) = E(\hat{\theta} - \theta)^2$$

$$E[\hat{\theta} - E(\hat{\theta}) + E(\hat{\theta}) - \theta]^2 = E[(\theta^2 - E(\hat{\theta}))^2 + B^2(\hat{\theta}) + 2B(\hat{\theta})(\theta - E(\hat{\theta})] = Var(\hat{\theta}) + B^2(\hat{\theta}) + 0.$$

Which is the $MSE(\hat{\theta})$.

Example: Suppose x_1, x_2, x_3 is a random sample of size 3. Then, $\bar{x}$ is unbiased on μ and

$$\frac{\sigma^2}{n} = \frac{\sigma^2}{3}.$$

Suppose that

$$\tilde{\mu} = \frac{2x_1 + x_1 + 2x_3}{5}.$$

Then,

$$E(\tilde{\mu}) = \frac{2\mu + \mu + 2\mu}{5} = \mu.$$

$$Var(\tilde{\mu}) = \frac{1}{5^2} Var(2x_1 + x_2 + 2x_3) = \frac{1}{5^2}(2^2\sigma^2 + \sigma^2 + 2^2\sigma^2) = \frac{9}{25}\sigma^2 > \frac{1}{3}\sigma^2.$$

In general,

$$\bar{x} = \frac{x_1 + x_2 + ... + x_n}{n}, \; \tilde{\mu} = \frac{a_1x_1 + a_2x_2 + ... + a_nx_n}{a_1 + a_2 + ... + a_n}.$$

Example: Suppose $X \sim N(\mu, \sigma^2)$. $x_1, ..., x_n$ is a random sample. μ and σ^2 are both unknown. Find the MSE estimator of σ^2 in the class of cS^2, where c is a constant.

$$s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2, \; E(s^2) = \sigma^2.$$

Suppose that,

$$\tilde{\sigma}^2 = cs^2.$$

Find $E(cs^2)$.

$$E(cs^2) = E(cs^2 - \sigma^2)^2.$$

Then,

$$\frac{(n-1)s^2}{\sigma^2} \sim \chi^2_{n-1}.$$

$$Y \sim \chi^2_{n-1}.$$

Therefore,

$$E(Y) = n-1, Var(Y) = 2(n-1).$$

$$Var\left[\frac{(n-1)s^2}{\sigma^2}\right] = 2(n-1).$$

Note that if a is a constant that,

$$Var(aX) = a^2 Var(X).$$

$$Var(s^2) = \frac{2\sigma^4}{n-1}.$$

$$MSE(cs^2) = E[cs^2 - \sigma^2]^2 = Var(cs^2 - \sigma) + [E(cs^2 - \sigma^2)]^2 = c^2 Var(s^2) + (c\sigma^2 - \sigma^2)^2 =$$

$$\sigma^4\left((c-1)^2 + \frac{2c^2}{n-1}\right) = K(c).$$

Then, minimize $K(c)$.

$$K'(c) = \sigma^4\left[2(c-1) + \frac{4c}{n-1}\right] = 0.$$

$$c = \frac{n-1}{n+1}.$$

The minimum MSE of

$$\sigma^2 = \frac{n-1}{n+1}s^2 = \frac{1}{n+1}\sum_{i=1}^{n}(x_i - \bar{x})^2.$$

is a biased estimator. s^2 is an unbiased estimator whereas the other is biased.

7.1.2 Method of Moments

Suppose that $X \sim f(x;\theta)$.

$$\mu(\theta) = E(X) = \int_{-\infty}^{\infty} x f(x;\theta)\,dx$$

is the first population moment. $x_1, ..., x_n$ is an iid sequence. Then, the sample mean is

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i.$$

The moment estimate of θ is

$$\mu(\theta) = \bar{x}.$$

The solution of this estimator is the moment estimate of θ. Suppose that

$$\theta = \theta_1, \theta_2.$$

$$m(\theta) = \bar{x}.$$

$$\mu_2'(\theta) = m_2' = E(x^2) = \int x^2 f(x;\theta)\,dx.$$

$$m_2' = \frac{1}{n}\sum_{i=1}^{n} x_i^2.$$

Example: Suppose $f(x;\theta) = \theta x^{\theta-1}, 0 < x < 1$. A moment estimate of θ is

$$\mu(\theta) = E(x) = \int_0^1 x\theta x^{\theta-1}\,dx = \theta\int_0^1 x^{\theta}\,dx = \left[\frac{\theta x^{\theta+1}}{\theta+1}\right]_0^1 = \frac{\theta}{1+\theta}.$$

$$\frac{\theta}{1+\theta} = \bar{x} \Rightarrow \theta = \bar{x} + \theta\bar{x} \Rightarrow \tilde{\theta} = \frac{\bar{x}}{1-\bar{x}}$$

We will learn the method of maximum likelihood which gives $\hat{\theta}$.

Example: Suppose $x \sim Gamma(\alpha,\theta)$. Then,

$$f(x|\alpha,\theta) = \frac{e^{\frac{-x}{\theta}} x^{\alpha-1}}{\Gamma(\alpha)\theta^{\alpha}}, x > 0.$$

$$E(x) = \alpha\theta,\ Var(x) = \alpha\theta^2$$

$$\alpha\theta = \bar{x},\ \alpha\theta^2 = m_2.$$

Therefore,

$$\tilde{\theta} = \frac{m_2}{\bar{x}},\ \alpha = \frac{\bar{x}^2}{m_2}.$$

Example: Suppose $x \sim N(\mu,\sigma^2)$.

$$\tilde{\mu} = \bar{x},\ \tilde{\sigma^2} = m_2.$$

7.1.3 Internal Estimation

Internal estimation is also called confidence intervals. Suppose $x \sim f(x;\theta)$ where $x_1, ..., x_n$ is an iid sequence. Let $\hat{\theta}$ be the point estimator of θ. Then, find $P(a < \theta < b) = 1 - \alpha$.

Example: $x \sim N(\mu,\sigma^2)$. Assume σ^2 is known. Find the internal estimator of μ. $x_1, x_2, ...x_n$ is an iid sequence. It is known that $\bar{x}$ is an estimator of μ.

$$\bar{x} \sim N\left(\mu, \frac{\sigma^2}{n}\right),\ Z = \frac{\sqrt{n}\bar{x} - \mu}{\sigma} \sim N(0,1).$$

$$1 - \alpha = P\left(-z_{\frac{\alpha}{2}} < Z < z_{\frac{\alpha}{2}}\right) \Rightarrow 1 - \alpha = P\left(\bar{x} - \frac{z_{\frac{\alpha}{2}}\sigma}{\sqrt{n}} < \mu < \bar{x} + \frac{z_{\frac{\alpha}{2}}\sigma}{\sqrt{n}}\right) \Rightarrow \left[\bar{x} - \frac{z_{\frac{z}{2}}\sigma}{\sqrt{n}}, \bar{x} + \frac{z_{\frac{\alpha}{2}}\sigma}{\sqrt{n}}\right]$$

is a $(1-\alpha)100\%$ confidence interval of μ. The interval length is given by the following equation, $\frac{2z_{\frac{\alpha}{2}}\sigma}{\sqrt{n}}$. The amount of error is given by the following equation, $\frac{z_{\frac{\alpha}{2}}\sigma}{\sqrt{n}}$.

Suppose the tails of the z statistic are uneven. A longer interval length given by the following expression should not be used: $(z_{\alpha_1} + z_{\alpha_2})\frac{\sigma}{\sqrt{n}}$.

Example: The GPA of students at ODU is $N(\mu,\sigma^2)$ with $\sigma = 0.3$. Based on a random sample of 16 students giving $\bar{X} = 2.7$, find a 95% confidence interval of μ.

$$\frac{\alpha}{2} = 0.025,\ z_{0.025} = 1.96.$$

Then,

$$2.7 \pm \frac{1.96(0.3)}{4} = [2.555, 2.845]$$

is the 95% confidence interval of the mean at ODU.

Suppose $X \sim N(\mu, \sigma^2)$ and σ^2 is unknown. The test statistic is

$$T = \frac{\sqrt{n}(\bar{X} - \mu)}{s} \sim t(n-1),\ 1 - \alpha = P(-t_{\alpha/2}(n-1) < T < t_{\alpha/2}(n-1)).$$

$r = n - 1$ if ever used.

$$1 - \alpha = P\left(\bar{X} - \frac{t_{\alpha/2}(n-1)s}{\sqrt{n}} < \mu < \bar{X} + \frac{t_{\alpha/2}(n-1)s}{\sqrt{n}}\right),$$

is the $(1-\alpha)100\%$ confidence interval. $\bar{X} \pm \frac{t_{\alpha/2}(n-1)s}{\sqrt{n}}$, is the interval. The length is, $\frac{2t_{\alpha/2}(n-1)s}{\sqrt{n}}$. To compare this statistic, the expected value of s should be used: $E(s^2) = \sigma^2$. Note that, $E(s) \neq \sigma$. Compare $\frac{2t_{\alpha/2}(n-1)E(s)}{\sqrt{n}}$ with $\frac{2z_{\alpha/2}\sigma}{\sqrt{n}}$. Suppose σ is unknown but $s = 0.35$. Find a 95% confidence interval for μ. $t_{0.025}(15) = 2.131$.

$$\bar{X} \pm \frac{t_{0.025}(15)s}{\sqrt{n}} = 2.7 \pm \frac{2.131(0.35)}{4} = [2.514, 2.886].$$

7.1.4 Means of Two Populations

Suppose we have two populations, Population I is $X \sim N(\mu_X, \sigma_X^2)$, and Population II is $Y \sim N(\mu_Y, \sigma_Y^2)$. Find a confidence interval for $\mu_X - \mu_Y$. It is assumed that, $x_1, x_2, ..., x_n$ and $y_1, y_2, ..., y_m$ are iid samples.

Case 1: σ_X, σ_Y are known. $\bar{X} - \bar{Y}$ is a point estimator of $\mu_X - \mu_Y$.

$$E(\bar{X} - \bar{Y}) = \mu_X - \mu_Y.$$

$$Var(\bar{X} - \bar{Y}) = Var(\bar{X}) + Var(\bar{Y}) = \frac{\sigma_X^2}{n} + \frac{\sigma_Y^2}{m} = \sigma_W^2.$$

Then, $\bar{X} - \bar{Y} \sim N(\mu_X - \mu_Y, \sigma_W^2)$. The test statistic is

$$\frac{\bar{X} - \bar{Y} - (\mu_X - \mu_Y)}{\sigma_W} \sim N(0, 1).$$

$$1 - \alpha = P(-z_{\alpha/2} < z < z_{\alpha/2}).$$

$$\bar{X} - \bar{Y} \pm z_{\alpha/2}\sigma_W = \bar{X} - \bar{Y} \pm z_{\alpha/2}\sqrt{\frac{\sigma_X^2}{n} + \frac{\sigma_Y^2}{m}}$$

is the $(1-\alpha)100\%$ confidence interval of $\mu_X - \mu_Y$.

Case 2: σ_X, σ_Y are unknown, but n, m are large (over 30). Then,

$$\bar{X} - \bar{Y} \pm z_{\alpha/2}\sqrt{\frac{s_X^2}{n} + \frac{s_Y^2}{m}}$$

is a $(1-\alpha)100\%$ confidence interval of $\mu_X - \mu_Y$. Note that,

$$s_X^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2,\ s_Y^2 = \frac{1}{m-1}\sum_{i=1}^{M}(y_i - \bar{y})^2.$$

Case 3: m, n are small, σ_X, σ_Y are unknown but are equal.

$$s_p^2 = \frac{(n-1)S_x^2 + (m-1)S_y^2}{n+m-2},$$

where S_p^2 is the pooled estimate of σ^2.

$$\frac{\bar{X} - \bar{Y} - (\mu_X - \mu_Y)}{S_p\sqrt{\frac{1}{n} + \frac{1}{m}}} \sim t(n+m-2).$$

The $(1-\alpha)100\%$ confidence interval for $\mu_X - \mu_y$ is

$$\bar{X} - \bar{Y} \pm t_{\alpha/2}(n+m-2)S_p\sqrt{\frac{1}{n} + \frac{1}{m}}.$$

Example: A random sample of 40 starting salaries of engineering graduates produced $\bar{X} = \$32,600$ and $S_x = \$4,172$. A random sample of 30 education graduates produced $\bar{Y} = \$24,900$ and $S_y = \$3,864$. Construct a 95% confidence interval for the difference of the two mean starting salaries. We are assuming Normal distributions.

$$32600 - 24900 \pm 1.96\sqrt{\frac{4172^2}{40} + \frac{2864^2}{30}} = 7700 \pm 1893 = [5807, 9593].$$

Example: Problem 6.2-14 in the text book.

$$n = 12,\ \bar{X} = 65.7,\ S_x = 4,\ m = 15,\ \bar{Y} = 68.2,\ S_y = 3.$$

Assume that $\sigma_x = \sigma_y = \sigma$. We must assume a Normal distribution of heights in both countries.

$$S_p^2 = \frac{16(11) - 9(14)}{11 + 14} = 12.08 \Rightarrow S_p = 3.48.$$

A 98% confidence interval is

$$65.7 - 68.2 \pm 2.485(3.48)\sqrt{\frac{1}{12} + \frac{1}{15}} = -2.5 \pm 3.35 \Rightarrow [-5.85, 0.85].$$

Case 4: n, m are small, $\sigma_x \neq \sigma_y$. Use Welche's T statistic for an approximate interval.

$$\frac{\bar{X} - \bar{Y} - (\mu_x - \mu_y)}{\sqrt{\frac{S_x^2}{n} + \frac{S_y^2}{m}}} \sim t(r),$$

where r is

$$\frac{\left(\frac{S_x^2}{n} + \frac{S_y^2}{m}\right)^2}{\frac{1}{n-1}\left(\frac{S_x^2}{n}\right)^2 + \frac{1}{m-1}\left(\frac{S_y^2}{m}\right)^2}.$$

$$\bar{X} - \bar{Y} \pm t_{\alpha/2}(r)\sqrt{\frac{S_x^2}{n} + \frac{S_Y^2}{m}}.$$

Example: 6.2-14 in the text book. If $\sigma_x \neq \sigma_y$, then $r = 19.95$. Choosing the largest integer for r, $r = 19$. $t_{0.01}(19) = 2.539$. Then,

$$65.7 - 68.2 \pm 2.539\sqrt{\frac{16}{12} + \frac{9}{15}} = -2.5 \pm 3.53 = [-6.03, 1.03].$$

7.2 Confidence Intervals

7.2.1 Confidence Intervals of σ^2

Assume $X \sim n(\mu, \sigma^2)$ and $x_1, x_2, ..., x_n$ is an iid sequence.

$$\tilde{\sigma}^2 = S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2.$$

$$\frac{(n-1)S^2}{\sigma^2} \sim \chi^2(n-1).$$

$$1 - \alpha = P(a < \chi^2(n-1) < b) = P\left(a < \frac{(n-1)S^2}{\sigma^2} < b\right) =$$

$$P\left(\frac{1}{b} < \frac{\sigma^2}{(n-1)S^2} < \frac{1}{a}\right) = P\left(\frac{(n-1)S^2}{b} < \sigma^2 < \frac{(n-1)S^2}{a}\right).$$

The confidence interval is

$$\left[\frac{(n-1)S^2}{b}, \frac{(n-1)S^2}{a}\right].$$

σ is

$$\left[\sqrt{\frac{(n-1)S^2}{b}}, \sqrt{\frac{(n-1)S^2}{a}}\right].$$

How to choose a and b. One way is

$$b = \chi_{\alpha/2}(r),\ a = \chi_{1-\alpha/2}(r),$$

where $r = n - 1$. The preferred way is the shortest confidence interval of σ given by

$$length = \sqrt{(n-1)S^2}\left(\frac{1}{\sqrt{a}} - \frac{1}{\sqrt{b}}\right).$$

Two constraints are:

1. the area is $1 - \alpha$.
2. minimize the length.

Use Table X on page 692 of the text book.

Example: 6.3-1 in the text book on page 356.

$$n = 13, \bar{X} = 18.97,\ (n-1)S^2 = \sum_{i=1}^{13}(x_i - \bar{x})^2 = 128.41.$$

Find a 90% confidence interval of σ.

$$a = \chi_{0.95}(12) = 5.226,\ b = \chi_{0.05}(12) = 21.03.$$

Then,

$$\left[\sqrt{\frac{(n-1)S^2}{b}}, \sqrt{\frac{(n-1)S^2}{a}}\right] = \left[\sqrt{\frac{128.01}{21.03}}, \sqrt{\frac{128.01}{5.226}}\right] = [2.22, 4.957].$$

The length is 2.485. The shortest length is $a = 5.94$, $b = 24.202$.

$$\left[\sqrt{\frac{128.41}{24.202}}, \sqrt{\frac{128.41}{5.94}}\right] = [2.303, 4.649].$$

The length this time is 2.346, which is shorter.

Suppose $X \sim N(\mu_x, \sigma_x^2), Y \sim N(\mu_y, \sigma_y^2)$. Find a confidence interval of $\frac{\sigma_x^2}{\sigma_y^2}$. Suppose that $\frac{S_x^2}{S_y^2}$ is an estimator of $\frac{\sigma_x^2}{\sigma_y^2}$. Then, $\frac{\frac{S_y^2}{\sigma_y^2}}{\frac{S_x^2}{\sigma_x^2}} \sim F(m-1, n-1)$.

$$1 - \alpha = P\left(a < \frac{S_y^2}{S_x^2}\sigma_x^2\sigma_y^2 < b\right) = P\left(a\frac{s_x^2}{s_y^2} < \frac{\sigma_x^2}{\sigma_y^2} < b\frac{S_x^2}{S_y^2}\right).$$

A $(1-\alpha)100\%$ confidence interval of $\frac{\sigma_x^2}{\sigma_y^2}$ is $\left[a\frac{S_x^2}{s_y^2}, b\frac{S_x^2}{S_y^2}\right]$ The simplest way to find a, b is to use $1-\alpha/2$ and $\alpha/2$ of $a = F_{1-\alpha/2}(m-1, n-1)$, $b = F_{\alpha/2}(m-1, n-1)$. Note that in the tables in the book, $1-\alpha/2$ points are not given. So, $F_{1-\alpha/2}(m-1, n-1) = \frac{1}{F_{\alpha/2}(m-1,n-1)}$.

7.2.2 Confidence Interval of the Binomial

Suppose $X \sim B(n, p)$. Then, a point estimate is $\hat{p} = \frac{x}{n}$, for large n.

$$\frac{X - np}{npq} = \frac{\frac{X}{n} - p}{\sqrt{\frac{pq}{n}}} = \frac{\hat{p} - p}{\sqrt{\frac{pq}{n}}} \sim N(0, 1).$$

$$E(X) = np, Var(X) = npq.$$

$$1 - \alpha = P(-z_{\alpha/2} z < z_{\alpha/2}) = P\left(-z_{\alpha/2} < \frac{\hat{p} - p}{\sqrt{\frac{pq}{n}}} < z_{\alpha/2}\right) = P\left(\frac{(\hat{p} - p)^2}{\frac{pq}{n}} \leq z_{\alpha/2}^2\right) =$$

$$P\left(p^2\left(1 + \frac{z_{\alpha/2}^2}{n}\right) - \left(2\hat{p} + \frac{z_0^2}{n}\right)p + \hat{p}^2 \leq 0\right).$$

$$p = \frac{\hat{p} + \frac{z_0^2}{n} \pm z_0\left(\frac{\hat{p}\hat{q}}{n} + \frac{z_0^2}{4n^2}\right)^{\frac{1}{2}}}{1 + \frac{z_0^2}{n}}.$$

A simpler version is given by,

$$\frac{\hat{p} - p}{\sqrt{\frac{\hat{p}\hat{q}}{n}}} \sim N(0, 1).$$

$$1 - \alpha = P\left(-z_{\alpha/2} < \frac{\hat{p} - p}{\sqrt{\frac{\hat{p}\hat{q}}{n}}} < z_{\alpha/2}\right) = P\left(\hat{p} - z_{\alpha/2}\sqrt{\frac{\hat{p}\hat{q}}{n}} < p < \hat{p} + z_{\alpha/2}\sqrt{\frac{\hat{p}\hat{q}}{n}}\right).$$

The $(1-\alpha)100\%$ confidence interval of p is $\hat{p} \pm z_{\alpha/2}\sqrt{\frac{\hat{p}\hat{q}}{n}}$.

Example: In a sample of 1150 voters, 565 are for candidate A in a presidential election. Find a 95% confidence interval of p, the proportion of all US voters who are for candidate A.

$$\hat{p} = \frac{565}{1150} = 0.491, z_{0.025} = 1.96.$$

$$\hat{p} \pm z_{0.025}\sqrt{\frac{\hat{p}\hat{q}}{n}} = 0.491 \pm (1.96)\sqrt{\frac{(0.491)(0.509)}{1150}} = 0.491 \pm 0.029 = [0.462, 0.520].$$

With the complicated formula, we get the same results.

Suppose two different populations $X \sim B(n, p_1)$, and $Y \sim B(n, p_2)$ are given. p_1 is the proportion of people who like a product and p_2 is the proportion of people who don't like the product. The confidence interval is derived as follow:

$$\hat{p}_1 = \frac{X}{n_1},\ \hat{p}_2 = \frac{Y}{n_2},\ E(\hat{p}_1 - \hat{p}_2) = p_1 = p_2.$$

$$Var(\hat{p}_1 + \hat{p}_2) = Var(\hat{p}_1) + Var(\hat{p}_2) = \frac{p_1q_1}{n_1} + \frac{p_2q_2}{n_2}.$$

For large n_1 and n_2,

$$\frac{\hat{p}_1 - \hat{p}_2 - (p_1 - p_2)}{\sqrt{\frac{\hat{p}_1\hat{q}_2}{n_1} + \frac{\hat{p}_2\hat{q}_2}{n_2}}} \sim N(0,1).$$

$$\hat{p}_1 - \hat{p}_2 \pm z_{\alpha/2}\sqrt{\frac{\hat{p}_1\hat{q}_1}{n_1} + \frac{\hat{p}_2\hat{q}_2}{n_2}}.$$

Example: Problem 6.4-10 on page 366 of the text book.

$$n_1 = 2100,\ n_2 = 1900,\ \hat{p}_1 = \frac{840}{2100} = 0.4,\ \hat{p}_2 = \frac{323}{1900} = 0.17.$$

A 90% confidence interval is derived as follow:

$$\sqrt{\frac{\hat{p}_1\hat{q}_1}{n_1} + \frac{\hat{p}_2\hat{q}_2}{n_2}} = 0.014.$$

Then,

$$0.4 - 0.17 \pm 1.645(0.014) = 0.23 \pm 0.023.$$

7.2.3 Sample Size

When designing an experiment, how large should the sample size n be?

Example: Suppose $X \sim N(\mu, \sigma^2)$. We are interested in estimating μ. How large should n be so that $\bar{X}$ is within 1 unit of μ with a probability of 0.95? the confidence interval of $\bar{X}$ is $\bar{X} \pm z_{0.025}\frac{\sigma^2}{\sqrt{n}}$. We want the latter part of the expression to be 1 unit. So, $z_{0.025}\frac{\sigma^2}{\sqrt{n}} = 1$. Solving for n, $n = 1.96^2\sigma^2$. The confidence interval is given by,

$$0.95 = P\left(-\frac{1}{\sqrt{n}\sigma} < \frac{\bar{X} - \mu}{\sigma/\sqrt{n}} < \frac{1}{\sqrt{n}\sigma}\right) \Rightarrow 0.95 = P(-1.96 < z < 1.96).$$

σ^2	1	2	5	10
n	4	8	19	38

With the Normal distribution, we must have the variance. With the Binomial distribution, we do not need the variance. To find a variance in a Normal distribution, perform a *pilot* experiment to estimate the variance. In general, $\epsilon = z_{\alpha/2}\frac{\sigma}{\sqrt{n}}$ is the maximum error in $\bar{X}$ for estimating μ with a probability of α. Suppose

ϵ is fixed. Then, we have $n = \frac{z^2_{\alpha/2}\sigma^2}{\epsilon^2}$.

Example: Suppose you want to estimate the GPA of students at ODU. You want $\bar{X}$ to be within 0.05 points of μ with the probability of 0.95. Find n. $\epsilon = 0.05, z_{0.025} = 1.96$. $n = \frac{(1.96)^2\sigma^2}{(0.05)^2}$.

σ^2	n
0.1	154
0.2	307

7.2.4 The Binomial Proportions

Suppose $X \sim B(n,p)$. The $(1-\alpha)100\%$ confidence interval of p is $\hat{p} \pm z_{\alpha/2}\sqrt{\frac{\hat{p}\hat{q}}{n}}$. The maximum error is $\epsilon = z_{\alpha/2}\sqrt{\frac{\hat{p}\hat{q}}{n}}$. Thus, $n = \hat{p}\hat{q}\frac{z^2_{\alpha/2}}{\epsilon^2}$. The maximum value is when $p = 1/2, pq = 1/4$. So, $n \le \frac{z^2_{\alpha/2}}{4\epsilon^2}$. Suppose that $\alpha = 0.05$ and $\epsilon = 0.03$. Then, $n \le \frac{(1.96)^2}{4(0.03)^2} = 1067$.

7.2.5 Homework and Answers

6.1-3: Given X_1, X_2, X_3, ..., X_n is an iid sequence and $X \sim b(1,p)$,

$$Y = \sum_{i=1}^{n} X_i \sim b(n,p).$$

(a) Show that $\bar{X} = \frac{Y}{n}$ is an unbiased estimator of p.

$$\bar{X} = \frac{Y}{n} = \frac{1}{n}\sum_{i=1}^{n} X_i.$$

According to page 155 of the text book, the expected value $E(Y)$ of a Binomial distribution is np. Thus, $E(Y) = np$. Then,

$$E(\bar{X}) = E\left(\frac{Y}{n}\right) = \frac{1}{n}E(Y) = \frac{np}{n} = p.$$

(b) Show that $Var(\bar{X}) = \frac{p(1-p)}{n}$. Looking at the variance,

$$Var(\bar{X}) = Var\left(\frac{Y}{n}\right) = \frac{1}{n^2}Var(Y) = \frac{np(1-p)}{n^2} = \frac{p(1-p)}{n}.$$

(c) Show that $E[\frac{\bar{X}(1-\bar{X})}{n}] = (n-1)[\frac{p(1-p)}{n^2}]$.

$$E\left[\frac{\bar{X}(1-\bar{X})}{n}\right] = E\left[\frac{\frac{Y}{n}(1-\frac{Y}{n})}{n}\right] = E\left[\frac{Y}{n^2}(1-\frac{Y}{n})\right] = E\left[\frac{Y}{n^2} - \frac{Y^2}{n^3}\right] = \frac{E(Y)}{n^2} - \frac{E(Y^2)}{n^3} =$$

$$\frac{np}{n^2} - \frac{\sigma^2+\mu^2}{n^3} = \frac{p}{n} - \frac{np(1-p)}{n^3} - \frac{n^2p^2}{n^3} = \frac{p}{n} - \frac{p(1-p)}{n^2} - \frac{p^2}{n} = \frac{np}{n^2} - \frac{p(1-p)}{n^2} - \frac{np^2}{n^2} =$$

$$\frac{np(1-p) - p(1-p)}{n^2} = \frac{(n-1)p(1-p)}{n^2}.$$

(d) Find the value of c so that $c\bar{X}(1-\bar{X})$ is an unbiased estimator of $\frac{p(1-p)}{n} = Var(\bar{X})$. The procedure to find c is to find $E(cS^2)$, set the derivative of $E(cS^2)$ equal to zero, and solve for c. Referring to page 156 of the text book, the variance of the Binomial distribution is $Var(Y) = E(Y^2) - [E(Y)]^2$.

6.1-4: Given $X_1, X_2, X_3, ..., X_n$ is an iid sequence with variance σ^2, show that

$$S^2 = \sum_{i=1}^{n} \frac{(X_i - \bar{X})^2}{n-1}$$

is an unbiased estimator of σ^2. To show that S^2 is an unbiased estimator means proving that $S^2 = \sigma^2$. The proof is as follow:

$$S^2 = \sum_{i=1}^{n} \frac{(X_i - \bar{X})^2}{n-1} = \sum_{i=1}^{n} \frac{X_i^2 - n\bar{X}^2}{n-1} = \sum_{i=1}^{n} \frac{\sigma^2 + \mu^2}{n-1} - \frac{n(\frac{\sigma^2}{n} + \mu^2)}{n-1} = \frac{n(\sigma^2 + \mu^2) - \sigma^2 - n\mu^2}{n-1} =$$

$$\frac{n\sigma^2 + n\mu^2 - \sigma^2 - n\mu^2}{n-1} = \frac{n\sigma^2 - \sigma^2}{n-1} = \frac{(n-1)\sigma^2}{(n-1)} = \sigma^2.$$

6.1-7: Let $X_1, X_2, ..., X_n$ be an iid sample where X is Gamma distributed. Let $\mu = \alpha\theta$ and $\sigma^2 = \alpha\theta^2$. Use method of moments to find estimates for α and θ.

$$m_1 = \frac{1}{n}\sum_{i=1}^{n} x_i = \bar{X} = \alpha\theta, \; m_2 = \frac{1}{n}\sum_{i=1}^{n} x_i^2.$$

The solution of α and θ relies on substituting $\bar{X}$ into the variance and solving for one or the other. Once either α or θ has been found, that expression can be substituted back into the variance to find the other parameter. Substituting $\bar{X}$ into the variance yields,

$$\sigma^2 = Var(X) = (\alpha\theta)\theta.$$

$$\bar{X}\theta = Var(X) \Rightarrow \theta = \frac{Var(X)}{\bar{X}}.$$

Using the previous expression for θ yields:

$$\alpha\left(\frac{Var(X)}{\bar{X}}\right)^2 = Var(X) \Rightarrow \alpha\frac{Var(X)^2}{\bar{X}^2} = Var(X) \Rightarrow \alpha = \frac{\bar{X}^2}{Var(X)}.$$

Note that the variance is given by

$$Var(X) = \frac{1}{n}\sum_i x_i^2 - \left(\frac{1}{n}\sum_i x_i^2\right)^2 = m_2 - m_1^2.$$

6.1-9: Let $f(x;\theta) = \theta x^{\theta-1}, 0 < x < 1, \theta \in \Omega = \theta : 0 < \theta < \infty$.

(a) For each of the following three sets of 10 observations from this distribution, calculate the value of the method of moments estimate for θ.

(i)	0.0256	0.3051	0.0278	0.8971	0.0739
	0.3191	0.7379	0.3671	0.9763	0.0102
(ii)	0.9960	0.3125	0.4374	0.7464	0.8278
	0.9518	0.9924	0.7112	0.2228	0.8609
(iii)	0.4698	0.3675	0.5991	0.9513	0.6049
	0.9917	0.1551	0.0710	0.2110	0.2154

Referring to page 337 in the text book, $\tilde{\theta} = \frac{\bar{X}}{1-\bar{X}}$.

$$m_1 = \frac{1}{n}\sum_{i-1}^{n} x_i,$$

For set 1:

$$m_1 = \frac{1}{10}\sum_{i=1}^{10} x_i = \frac{3.7401}{10} = 0.37401.$$

$$\tilde{\theta} = \frac{0.37401}{1-0.37401} = 0.597469608.$$

For set 2:

$$m_1 = \frac{1}{10}\sum_{i=1}^{10} x_i = \frac{7.0592}{10} = 0.70592.$$

$$\tilde{\theta} = \frac{0.70592}{1-0.70592} = 2.40043525.$$

For set 3:

$$m_1 = \frac{1}{10}\sum_{i=1}^{10} x_i = \frac{4.6368}{10} = 0.46368.$$

$$\tilde{\theta} = \frac{0.46368}{1-0.46368} = 0.864558472$$

(b) For each set of data, sketch the empirical and theoretical distribution function(using your estimate of the value of θ) on the same graph. The cdf is $F(x,\theta) = x^{\theta}$ by integrating the pdf. The insert on the next page contains the graphs. Note: the graphs do not appear together in the same diagram because that is not possible in Lotus 1-2-3. Sorry.

6.1-17: As a clue to the amount of organic waste in Lake Macatawa(see Example 6.1-9), a count was made of the number of bacteria colonies in 100 milliliters of water. The number of colonies, in hundreds, for $n = 30$ samples of water from the east basin yielded

93	140	8	120	3	120
33	70	91	61	7	100
19	98	110	23	14	94
57	9	66	53	28	76
58	9	73	49	37	92

Find an approximate 90% confidence interval for the mean number of colonies in 100 milliliters of water in the east basin, μ_E. $\alpha = 0.10$, $z_{\frac{\alpha}{2}} = z_{0.05} = 1.645$. Since there are 30 samples, the z statistic is appropriate.

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i = \frac{1}{30}\sum_{i=1}^{30} x_i = \frac{1181}{30} = 60.36666.$$

$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n} x_i^2 - \bar{x}^2.$$

$$S^2 = \frac{1}{29}\sum_{i=1}^{30} x_i^2 - \bar{x}^2 = \frac{154851 - 109324.0333}{29} = 1517.57.$$

The confidence interval is given by the following expression:

$$\bar{x} \pm z_{0.05}\left(\frac{S}{\sqrt{n}}\right) = 60.36667 \pm 1.645\left(\frac{39.6219}{\sqrt{30}}\right).$$

Therefore, the confidence interval is [48.46684, 72.2665].

6.2-1: Let X equal the thickness of peppermint gum that is manufactured for vending machines. Assume that the distribution of X is $N(\mu, \sigma^2)$. The target thickness is 7.5 hundredth of an inch. The following $n = 10$ thicknesses, in hundredth of an inch, were made on pieces of gum that were selected randomly from the production line:

7.50	7.55	7.55	7.40	7.45	7.35	7.45	7.45	7.45	7.5

(a) Give point estimates of μ and σ.

$$\bar{x} = \frac{1}{10}\sum_{i=1}^{10} x_i = \frac{74.65}{10} = 7.465.$$

$$S^2 = \frac{1}{9}\sum_{i=1}^{10} x_i^2 - \bar{x}^2 = \frac{557.2975 - 557.26225}{9} = 0.00391667 \Rightarrow S = 0.062583304.$$

(b) Find a 95% confidence interval for μ. Since X is known to have a Normal distribution and σ^2 is unknown, and the sample size is small, the t statistic should be used. $t_{0.025}(9) = 2.262$, gives a 95% confidence interval for μ.

$$7.465 \pm 2.262\left(\frac{0.062583304}{\sqrt{10}}\right) = [7.4202, 7.5098]$$

6.2-9: Let $X_1, X_2, ..., X_n$ be a random sample of size n from the Normal distribution $N(\mu, \sigma^2)$. Calculate the expected length of a 95% confidence interval for μ assuming that $n = 5$ and the variance is known and unknown.

(a) When the variance is known, the z statistic can be used. The 95% confidence interval is

$$P\left(-z_{\frac{\alpha}{2}} \leq \frac{\bar{X}-\mu}{\sigma/\sqrt{n}} \leq z_{\frac{\alpha}{2}}\right) = 1-\alpha$$

$$P\left(-z_{0.025} \leq \frac{\bar{X}-\mu}{\sigma/\sqrt{5}} \leq z_{0.025}\right) = 1-0.95$$

$$P\left(-1.96 \leq \frac{\bar{X}-\mu}{\sigma/\sqrt{5}} \leq 1.96\right) = 0.05$$

$$P\left(\bar{X} - 1.96\left(\frac{\sigma}{\sqrt{5}}\right) \leq \mu \leq \bar{X} + 1.96\left(\frac{\sigma}{\sqrt{5}}\right)\right) = 0.05$$

$$\left[\bar{X} - 1.96\left(\frac{\sigma}{\sqrt{5}}\right), \bar{X} + 1.96\left(\frac{\sigma}{\sqrt{5}}\right)\right].$$

$$2\left(\frac{1.96\sigma}{\sqrt{5}}\right) = 1.7531\sigma.$$

(b) Given the hint, $E(s) = \frac{1}{\chi^2_{0.90}} = \frac{\sigma}{1.064}$. When the variance is unknown, the t statistic should be used. The 95% confidence interval is

$$1-\alpha = P\left(-t_{\frac{\alpha}{2}}(n-1) \leq \frac{\bar{X}-\mu}{S/\sqrt{n}} \leq t_{\frac{\alpha}{2}}(n-1)\right)$$

$$0.05 = P\left(-t_{0.025}(4) \leq \frac{\bar{X}-\mu}{S/\sqrt{5}} \leq t_{0.025}(4)\right)$$

$$0.05 = P\left(-2.776 \leq \frac{\bar{X}-\mu}{S/\sqrt{5}} \leq 2.776\right)$$

$$0.05 = P\left(\bar{X} - 2.776\left(\frac{S}{\sqrt{5}}\right) \leq \mu \leq \bar{X} + 2.776\left(\frac{S}{\sqrt{5}}\right)\right)$$

$$\left[\bar{x} - 2.776\left(\frac{E(s)}{\sqrt{5}}\right), \bar{x} + 2.776\left(\frac{E(s)}{\sqrt{5}}\right)\right]$$

$$\left[\bar{x} - 2.776\left(\frac{\sigma}{1.064\sqrt{5}}\right), \bar{x} + 2.776\left(\frac{\sigma}{1.064\sqrt{5}}\right)\right].$$

The interval length is

$$2\left(\frac{2.776\sigma}{1.064\sqrt{5}}\right) = 2.333581\sigma.$$

6.2-10: Students took $n = 35$ samples of water from the east basin of Lake Macatawa(see Example 6.1-9) and measured the amount of sodium in parts per million. For their data they calculated $\bar{x} = 24.11$ and $s^2 = 24.44$. Find an approximate 90% confidence interval for μ, the mean of the amount of sodium in parts per million. Use $z_{\frac{\alpha}{2}} = z_{0.05} = 1.645$. The confidence interval is

$$\bar{x} \pm 1.645\left(\frac{s}{\sqrt{n}}\right) = 24.11 \pm 1.645\left(\frac{4.94368}{\sqrt{35}}\right) = [22.7354, 25.4846].$$

6.2-12: The length of life of brand X light bulbs is assumed to be $N(\mu_X, 784)$. The length of life of brand Y light bulbs is assumed to be $N(\mu_Y, 627)$ and independent of that of X. If a random sample of $n = 56$ brand X light bulbs yielded a mean of $\bar{x} = 937.4$ hours and a random sample of $m = 57$ brand Y light bulbs yielded a mean of $\bar{y} = 988.9$ hours, find a 90% confidence interval for $\mu_X - \mu_Y$.

$$W = \bar{X} - \bar{Y} \sim N\left(\mu_X - \mu_Y, \frac{\sigma_X^2}{n} + \frac{\sigma_Y^2}{m}\right).$$

$$\sigma_W = \sqrt{\frac{\sigma_X^2}{n} + \frac{\sigma_Y^2}{m}} = \sqrt{\frac{784}{56} + \frac{627}{57}} = 5.$$

$\bar{x} - \bar{y} = 937.4 - 988.9 = -51.5.$

$1.645\sigma_W = 1.645(5) = 8.225.$

The 90% confidence interval is [-51.5-8.225, -51.5+8.225] = [-59.725, -43.275].

6.2-13: Let $X_1, X_2, ..., X_5$ be a random sample of SAT mathematics scores, assumed to be $N(\mu_X, \sigma^2)$, and let $Y_1, Y_2, ..., Y_8$ be an independent random sample of SAT verbal scores, assumed to be $N(\mu_Y, \sigma^2)$. If the following data are observed, find a 90% confidence interval for $\mu_X - \mu_Y$:

$x_1 = 644$	$x_2 = 493$	$x_3 = 532$	$x_4 = 462$	$x_5 = 565$
$y_1 = 623$	$y_2 = 472$	$y_3 = 492$	$y_4 = 661$	$y_5 = 540$
$y_6 = 502$	$y_7 = 549$	$y_8 = 518$		

$$\bar{x} = \frac{1}{5}\sum_{i=1}^{5} x_i = \frac{2696}{5} = 539.2.$$

$$s_X^2 = \frac{1}{4}\sum_{i=1}^{5} x_i^2 - \bar{x}^2 = \frac{1473478 - 5(539.2)^2}{4} = 4948.7.$$

$$\bar{y} = \frac{1}{8}\sum_{i=1}^{8} y_i = \frac{4357}{8} = 544.625.$$

$$s_Y^2 = \frac{1}{7}\sum_{i=1}^{8} y_i^2 - \bar{y}^2 = \frac{2403227 - 8(544.625)^2}{7} = 4327.982.$$

$$s_P = \sqrt{\frac{(n-1)s_X^2 + (m-1)s_Y^2}{n+m-2}} = \sqrt{\frac{4(4948.7) + 7(4327.982)}{5+8-2}} = 67.481.$$

Since we only have estimates for σ^2, use the t distribution.

$$t_0 = t_{\frac{\alpha}{2}}(n+m-2) = t_{0.05}(11) = 1.796.$$

The 90% confidence interval of $\mu_X - \mu_Y$ is given by

$$\bar{x} - \bar{y} \pm t_0 s_P \sqrt{\frac{1}{n} + \frac{1}{m}}$$

So,

$$539.2 - 544.625 \pm 1.796(67.481)\sqrt{\frac{1}{5} + \frac{1}{8}} = 539.2 - 544.625 \pm 69.09 = [-74.515, 63.665].$$

6.2-15: [*Medicine and Science in Sports and Exercise* (January 1990)] Let X and Y equal, respectively, the blood volumes in milliliters for a male who is a paraplegic and participates in vigorous physical activities and a male who is able-bodied and participates in normal activities. Assume that $X \sim N(\mu_X, \sigma^2)$ and $Y \sim N(\mu_Y, \sigma^2)$. Using the following $n = 7$ observations of X :

1612	1352	1456	1222	1560	1456	1924

and $m = 10$ observations of Y :

1082	1300	1092	1040	910
1248	1092	1040	1092	1288

(a) Give a point estimate for $\mu_X - \mu_Y$.

$$\bar{x} = \frac{1}{7}\sum_{i=1}^{7} x_i = \frac{10582}{7} = 1511.7143.$$

$$\bar{y} = \frac{1}{10}\sum_{i=1}^{10} y_i = \frac{11184}{10} = 1118.4.$$

$\mu_X - \mu_Y = 1511.7143 - 1118.4 = 393.3143.$

(b) Find a 95% confidence interval for $\mu_X - \mu_Y$. Since the variances σ_X^2 and σ_Y^2 might not be equal, use Welch's T.

$$r = \frac{\left(\frac{49670.2071}{7} + \frac{15297.6}{10}\right)^2}{\frac{1}{6}\left(\frac{49670.2071}{7}\right)^2 + \frac{1}{9}\left(\frac{15297.6}{10}\right)^2} = \frac{74399317.04}{8391596.848 + 260018.4064} = 8.59947.$$

$$s_X^2 = \frac{1}{6}\sum_{i=1}^{7} x_i^2 - \bar{x}^2 = \frac{16294980 - 7(1511.7142)^2}{6} = 49670.2071.$$

$$s_Y^2 = \frac{1}{9}\sum_{i=1}^{10} y_i^2 - \bar{y}^2 = \frac{12645864 - 10(1118.4)^2}{9} = 15297.6.$$

$t_{0.025}(8) = 2.306.$

The confidence interval is

$$\bar{x} - \bar{y} \pm t_{\frac{\alpha}{2}}\sqrt{\frac{s_x^2}{n} + \frac{s_y^2}{m}} = 1511.7143 - 1118.4 \pm 2.306(92.873591) =$$

$$1511.7143 - 1118.4 \pm 214.1665 = [179.1475, 607.4805].$$

7.3 Maximum Likelihood Estimator

There are two ways to find an estimator of the parameter θ.

1. Method of Moments

2. Method of Maximum Likelihood

Example: Suppose $x_1, x_2, ..., x_n$ is a set of Bernoulli trials.

$$f(x|\theta) = \theta^x (1-\theta)^{1-x}, x = 0, 1, 2, ...$$

The joint pdf of the sample is

$$P(X_1 = x_1, X_2 = x_2, ..., X_n = x_n) = \prod_{i=1}^{n} f(x;\theta) = P(X_1 = x_1)P(X_2 = x_2)\cdots P(X_n = x_n) =$$

$$\prod_{i=1}^{n} \theta^{x_i}(1-\theta)^{1-x_i} = \theta^{\sum x_i}(1-\theta)^{n-\sum x_i} = \theta^{n\bar{X}}(1-\theta)^{n-n\bar{X}} = L(\theta|x).$$

Maximizing $L(\theta|x)$ is the same as the maximum of $\log L(\theta|x)$. So,

$$\log L = n\bar{X}\log\theta + n(1-\bar{X})\log(1-\theta),$$

$$\frac{\partial \log L}{\partial\theta} = \frac{n\bar{X}}{\theta} + \frac{n(1-x)}{1-\theta} = 0.$$

Thus, $\hat{\theta} = \bar{X}$. The moment estimate $E(X) = 1\theta + 0(1-\theta) = \theta$.

$$\tilde{\theta} = \bar{X} = \frac{1}{n}\sum_{i=1}^{n} x_i.$$

In general, MLE's are better estimators when they are different from the moment estimators.

Example: $X \sim Exp(\theta)$. Then,

$$f(x|\theta) = \frac{1}{\theta}e^{-\frac{x}{\theta}}.$$

$x_1, x_2, ..., x_n$ is an iid sequence.

$$L(\theta|x) = \prod_{i=1}^{n}\frac{1}{\theta}e^{-\frac{x_i}{\theta}} = \frac{1}{\theta^n}e^{-\frac{\sum x_i}{\theta}} = \frac{1}{\theta^n}e^{-\frac{n\bar{X}}{\theta}}.$$

$$\log L = -n\log\theta - \frac{n\bar{X}}{\theta},$$

$$\frac{\partial L}{\partial\theta} = -\frac{n}{\theta} + \frac{n\bar{X}^2}{\theta^2} = 0.$$

Thus, $\hat{\theta} = \bar{X}$.

Example:

$$f(x|\theta) = \frac{1}{\theta}, 0 < x < \theta, \theta > 0.$$

Suppose $x_1, x_2, ..., x_n$ is an iid sequence. Then,

$$L(\theta|x) = \prod_{i=1}^{n} f(x|\theta) = \prod_{i=1}^{n}\frac{1}{\theta} = \frac{1}{\theta^n}.$$

$$\log L = -n\log\theta.$$

$$\frac{\partial L}{\partial\theta} = -\frac{n}{\theta} = 0.$$

Since this fails to produce meaningful results, look at the graph of θ vs $L(\theta|x)$. As one can see, the $MLE = \hat{\theta} = x_{(m)}$. The moment estimator is given by $E(X) = \frac{\theta}{2} = \bar{X}$. Thus $\tilde{\theta} = 2\bar{X}$, which is different from the MLE. This is not even acceptable because of the original condition on x. The distribution of $x_{(m)}$ is needed.

$$y = x_{(m)},$$

$$g(y|\theta) = nf(y|\theta)F(y|\theta)^{n-1}.$$

For a uniform distribution,

$$f(y|\theta) = \frac{y}{\theta},$$

$$g(y|\theta) = n\frac{1}{\theta}\left(\frac{y}{\theta}\right)^{n-1} = \frac{ny^{n-1}}{\theta^n}, 0 < y < \theta.$$

$$E(Y) = \frac{n}{\theta^n}\int_0^\theta yy^{n-1}\,dy = \frac{n}{\theta^n}\int_0^\theta y^n\,dy = \frac{n}{n+1}\theta.$$

$$E(\hat{\theta}) = E(x_{(m)}) = \frac{n}{n+1}\theta,$$

which is a biased estimator. An unbiased estimator is given by

$$\hat{\theta}^* = \frac{n=1}{n}x_{(m)}.$$

$$E(\hat{\theta}^*) = \frac{n+1}{n}E(x_{(m)}) = \theta.$$

Example: Suppose $X \sim Poisson(\theta)$. Then,

$$f(x|\theta) = \frac{e^{-\theta}\theta^x}{x!}, x = 0, 1, 2, ...$$

$$E(X) = \theta$$

The moment estimate of $\tilde{\theta}$ is $\bar{X}$. The MLE is derived as follow:

$$\prod_{i=1}^n \frac{e^{-\theta}\theta^{x_i}}{x_i!} = \frac{e^{-n\theta}\theta^{\sum x_i}}{\prod x_i!} = \frac{e^{-n\theta}\theta^{n\bar{X}}}{c},$$

where $c = \prod x_i!$.

$$\log L = -n\theta + n\bar{X}\log\theta - \log c.$$

$$\frac{\partial L}{\partial\theta} = -n + \frac{n\bar{X}}{\theta} = 0.$$

$$\hat{\theta} = \bar{X},$$

which is the same as the moment estimate of θ.

7.3.1 The MLEs of Two Parameters

Suppose there are two parameters such that, $X \sim N(\theta_1, \theta_2)$, where $\theta_2 = Var(X)$. Suppose $x_1, x_2, ..., x_n$ is an iid sequence. Then,

$$f(x|\theta) = \frac{1}{\sqrt{2\pi\theta_2}}e^{-\left(\frac{x-\theta_1}{2\theta_2}\right)^2}.$$

$$L(\theta|x) = \prod_{i=1}^n f(x|\theta) = \frac{1}{2n\pi\theta_2}e^{-\frac{\sum(x_i-\theta_1)^2}{2\theta_2}}.$$

$$\log L = c - \frac{n}{2}\log\theta_2 - \frac{\sum(x_i-\theta_1)^2}{2\theta_2}.$$

$$\frac{\partial \log L}{\partial \theta_1} = -2(-1)\frac{\sum(x_i-\theta_1)}{2\theta_2} = 0.$$

Thus,

$$\theta_1 = \bar{X}.$$

$$\frac{\partial \log L}{\partial \theta_2} = -\frac{n}{2\theta_2} - (-1)\frac{\sum(x_i-\theta_1)^2}{2\theta_2^2} = 0.$$

Thus,

$$\theta_2 = \frac{1}{n}\sum_{i=1}^{n}(x_i-\theta_1)^2.$$

Finally,

$$\hat{\theta}_1 = \bar{X},\, \hat{\theta}_2 = \frac{1}{n}\sum_{i=1}^{n}(x_i-\bar{x})^2.$$

Note that θ_2 is biased.

$$E(\hat{\theta}_2) = E\left(\frac{1}{n}\sum_{i=1}^{n}(x_i-\bar{X})^2\right) = \frac{n-1}{n}E\left(\frac{1}{n-1}\sum_{i=1}^{n}(x_i-\bar{X})^2\right).$$

$\frac{n-1}{n}\theta_2$ is the bias.

7.3.2 Rao-Cramer Inequality

$X \sim f(x|\theta)$, where $\hat{\theta}$ is an unbiased estimator of θ based on $x_1, x_2, ..., x_n$. To find the lower bound on the estimator of the variance,

$$I(\theta) = \frac{\partial^2 \log f(x|\theta)}{\partial\theta^2} = -E\left(\frac{\partial^2 \log f(x|\theta)}{\partial\theta^2}\right) = E\left(\frac{\partial \log f)}{\partial\theta}\right)^2.$$

Theorem: Let $\hat{\theta}$ be an unbiased estimator of θ based on a sample of size n. Then,

$$Var(\hat{\theta}) \geq \frac{1}{nI(\theta)}.$$

Example: Suppose $X \sim Poisson(\theta)$.

$$f(x|\theta) = \frac{e^{-\theta}\theta^x}{x!}.$$

$$\log f = -\theta + x\log\theta - \log x!$$

$$\frac{\partial \log f}{\partial\theta} = -1 + \frac{x}{\theta},$$

$$-\frac{\partial^2 \log f}{\partial\theta^2} = \frac{x}{\theta^2}.$$

$$I(\theta) = -E\left(\frac{\partial^2 \log f}{\partial\theta^2}\right) = \frac{1}{\theta^2}E(X) = \frac{\theta}{\theta^2} = \frac{1}{\theta}.$$

Then, the lower bound is $\frac{1}{nI(\theta)} = \frac{\theta}{n}$. The MLE $\hat{\theta} = \bar{X}$ is an unbiased estimator for θ, which is the lower bound.

7.3.3 Chebyshev's Theorem

For any $k > 1$,

$$P\left(\frac{|x-\mu|}{\sigma} \geq k\right) \leq \frac{1}{k^2} = P\left(\frac{|x-\mu|}{\sigma} \leq k\right) \geq 1 - \frac{1}{k^2} = P(\mu - k\sigma < x < \mu + k\sigma) \geq 1 - \frac{1}{k^2}.$$

k is the standard deviation. The distribution does not need to be known for the theorem to work. The above expression can also be thought of as a confidence interval of X. The confidence interval of μ if σ is known and the distribution of X is unknown is,

$$E(\bar{X}) = \mu, Var(\bar{X}) = \frac{\sigma^2}{n}.$$

$$P\left(\mu - \frac{2\sigma}{\sqrt{n}} < \bar{X} < \mu + \frac{2\sigma}{\sqrt{n}}\right) \geq 0.75 = P\left(\bar{X} - \frac{2\sigma}{\sqrt{n}} < \mu < \bar{X} + \frac{2\sigma}{\sqrt{n}}\right) \geq 0.75.$$

Example: Police are interested in the age profile of serial killers. Based on 15 solved cases of serial killers in the US, the average age is 28.5 years old with a standard deviation of 2 years. Give a 75% confidence interval for the age of the serial killer. X is the age of the serial killer.

$$P(\mu - 2\sigma < X < \mu + 2\sigma) \geq 0.75.$$

$$P(28.5 \pm 2(2)) = [24.5, 32.5].$$

7.4 Testing of Hypotheses about Parameters

Example: Suppose X is the life of an electrical heater. The distributor says $X \sim N(50, \sigma^2)$, and the producer says $X \sim N(60, \sigma^2)$. Assume that σ is known. The hypotheses are stated as follow: $H_0 : \mu = 50$. versus $H_1 : \mu = 60$. Which hypothesis is more likely to be true?

Suppose that $x_1, x_2, ..., x_n$ is a random sample.

$$\hat{\mu} = \bar{X}, \bar{X} \sim N\left(50, \frac{\sigma^2}{n}\right), \bar{X} \sim N\left(60, \frac{\sigma^2}{n}\right).$$

Decision	H_0 true	H_1 true
Reject H_0	Type I Error	Correct
Reject H_1	Correct	Type II Error

$$\alpha = P(\text{Reject } H_0 | H_0 \text{ true}) = P(\bar{X} \geq c | H_0).$$

$$\beta = P(\text{Reject } H_1 | H_1 \text{ true}) = P(\bar{X} < c | H_1).$$

1. As α decreases, β increases for a fixed n.
2. If c is the same for all n then both α and β decrease as n increases.

How to find c.

Example: Find c for $\sigma = 5$ and $\alpha = 0.05$.

$$0.05 = P(\bar{X} > c | H_0) = P\left(\frac{\bar{X} - 50}{5/\sqrt{n}} > \frac{c - 50}{5/\sqrt{n}} | H_0\right)$$

$$0.05 = P\left(z > \frac{(c-50)\sqrt{n}}{5}\right) = P(z > 1.645).$$

Then,

$$\frac{(c-50)\sqrt{n}}{5} = 1.645 \Rightarrow c = \frac{8.2}{\sqrt{n}} + 50.$$

The test is reject H_0 if $\bar{X} > c = \frac{8.5}{\sqrt{n}} + 50$ or reject H_0 if $\frac{(\bar{X}-50)\sqrt{n}}{5} > z_{0.05} = 1.645$. 1.645 is called the *critical point* for H_0. The power of a test is given by $P(\text{Reject } H_0|H_1)$, when H_1 is true.

7.4.1 Power Tests

Example: Suppose we have the following hypothesis, $H_0 : \mu = 50$ versus $H_1 : \mu > 50$. Reject H_0 if $\bar{X} > c$, $c = \frac{8.20}{n} + 50$. Suppose that $n = 16, c = 52.05, \alpha = 0.05$. Find β and the power.

$$\beta = P(\text{Reject } H_1|H_1) = P(\bar{X} < 52.05|\mu_1) = P\left(z \leq \frac{52.05 - \mu_1}{1.25}\right).$$

μ_1	53	54	55
z	-0.76	-1.56	-2.36
β	0.2236	0.0595	0.0091
Power$=1-\beta$	0.7764	0.9405	0.9909

7.4.2 Testing About Proportions

Example: p is the proportion of Democrats in Norfolk. Suppose the test is as follow: $H_0 : p = 0.5$ versus $H_1 : p < 0.5$. Take a sample of size n. y equals the number of democrats out of n. Then, $Y \sim \textit{Binomial}(n, p)$. Reject H_0 if $Y \leq c$.

$$\alpha = P(\text{Reject } H_0|H_0) = P(Y \leq c|p = 0.5) = \sum_{y=0}^{2} \left(\begin{array}{c} n \\ y \end{array}\right) \quad \left(\tfrac{1}{2}\right)^n$$

For $n = 10$, $c = 2$, find α.

$$\alpha = \sum_{y=0}^{2} \left(\begin{array}{c} 10 \\ y \end{array}\right) \quad \left(\tfrac{1}{2}\right)^{10}$$

Then, $c = 1$, and $\alpha = 0.0007$. In the discrete case we can only come close to $\alpha = 0.05$ at $c = 2$. For large n, $H_0 : p = p_0$, $\hat{p} = \frac{Y}{n}$, $z_0 = \frac{\hat{p} - p_0}{\sqrt{\frac{p_0 q_0}{n}}} \sim N(0, 1)$.

H_1	Reject H_0
$p > p_0$	$z > z_\alpha$
$p < p_0$	$z < x_\alpha$
$p \neq p_0$	$\|z\| > z_{\alpha/2}$

z is the test statistic.

Example: Problem 7.1-3 on page 399 of the text book. $H_0 : p = 0.08$ versus $H_1 : p < 0.08$. Given $n = 100$, reject H_0 if $y \leq 6$. Find α.

- The exact value of α is given by

$$P(y \leq 6) = \sum_{y=0}^{6} \left(\begin{array}{c} 100 \\ y \end{array}\right) \quad (0.08)^y \quad (0.92)^{100-y} \quad = 0.3032$$

- The Poisson approximation of α is, $\lambda = np_0 = 100(0.08) = 8$.

$$\alpha = P(y \le 6|\lambda = 8) = \sum_{y=0}^{6} \frac{e^{-8}8^y}{y!} = 0.313.$$

- The Normal approximation of α is

$$\alpha = P(y \le 6) = P(y \le 6.5) = P\left(\frac{y-8}{\sqrt{npq}} \le \frac{6.5-8}{2.713}\right) = P(z \le -0.55) = 0.2912.$$

Find β for $H_1 : p = 0.04$.

$$P(\text{Reject } H_1|p = 0.04) = P(y > 6|p = 0.04) = 1 - P(y \le 6|p = 0.04) = 1 - \sum_{y=0}^{6} \frac{e^{-4}4^y}{y!} = 0.111.$$

7.4.3 Testing About Two Proportions

Suppose we wish to test about two proportions. $X \sim Bin(n_1, p_1), Y \sim Bin(n_2, p_2)$. We wish to test, $H_0 : p_1 = p_2$. Assume large n_1 and n_2. The Normal approximation must be used. Under H_0, $\hat{p}_1 = \frac{x}{n_1}$, $\hat{p}_2 = \frac{y}{n_2}$.

$$\frac{\hat{p}_1 - \hat{p}_2 - (p_1 - p_2)}{\sqrt{\frac{p_1q_1}{n_1} + \frac{p_2q_2}{n_2}}} \sim N(0,1), \quad \frac{\hat{p}_1 - \hat{p}_2}{\sqrt{pq\left(\frac{1}{n_1} + \frac{1}{n_2}\right)}} \sim N(0,1)$$

because H_0 is true. Then,

$$z = \frac{\hat{p}_1 - \hat{p}_2}{\sqrt{\hat{p}\hat{q}\left(\frac{1}{n_1} + \frac{1}{n_2}\right)}}, \ \hat{p} = \frac{x+y}{n_1+n_2}.$$

H_1	Reject if
$p_1 > p_2$	$z > z_\alpha$
$p_1 < p_2$	$z < -z_\alpha$
$p_1 \neq p_2$	$\lvert z\rvert > z_{\alpha/2}$

Example: Newsweek — 1988. Heart attack among doctors. Study the effect of aspirin. For the placebo group $n_1 = 11000$ and for the aspirin group $n_2 = 11000$. In the placebo group there were 18 deaths and 189 heart attacks. In the aspirin group there were 4 deaths and 104 heart attacks. The hypothesis test is stated as follow: $H_0 : p_1 = p_2$ versus $H_1 : p_1 > p_2$.

$$\hat{p}_1 = \frac{18}{11000} = 0.0016, \hat{p}_2 = \frac{4}{11000} = 0.0004.$$

The test statistic is

$$z = \frac{\hat{p}_1 - \hat{p}_2}{\sqrt{\frac{\hat{p}_1\hat{q}_1}{n_1} + \frac{\hat{p}_2\hat{q}_2}{n_2}}} = 2.82.$$

Reject H_0 if $z > z_\alpha$. For $\alpha = 0.05$, $p = P(z > 2.82) = 0.00251$. Thus, there is a significant difference. The null hypothesis is rejected.

Example: Immunization rates. Suppose p_1 is the probability that a child is immunized in Hampton, and p_2 is the probability that a child is immunized in Norfolk. Given intervention in Norfolk(children are required to be immunized), the hypothesis test is stated as: $H_0 : p_1 = p_2$ versus $H_1 : p_1 > p_2$. $n_1 = 200, n_2 = 175, X = 142, Y = 107$. Then, $\hat{p}_1 = 0.71, \hat{p}_2 = 0.61 \Rightarrow \hat{p} = 0.664$. The test statistic is $z = \frac{0.71-0.61}{\sqrt{0.664(0.336)\left(\frac{1}{200}+\frac{1}{175}\right)}} \Rightarrow z = 2.045$. Suppose $\alpha = 0.05$. Since $2.045 > 1.645$, reject H_0.

7.4.4 Homework

6.3-2 A random sample of $n = 9$ wheels of cheese yielded the following weights in pounds, assumed to be $N(\mu, \sigma^2)$:

21.50	18.95	18.55	19.40	19.15
22.35	22.90	22.20	23.10	

(a) Give a point estimate of σ.

$$\bar{x} = \frac{1}{9}\sum_{i=1}^{9} x_i = \frac{188.1}{9} = 20.9.$$

$$8s^2 = \sum_{i=1}^{9}(x_i - \bar{x})^2 = 27.63 \Rightarrow s = \sqrt{\frac{27.63}{8}} = 1.8584.$$

(b) Find a 95% confidence interval for σ. The following format will give the confidence interval:

$$\left[\sqrt{\frac{(n-1)s^2}{b}}, \sqrt{\frac{(n-1)s^2}{a}}\right].$$

a and b will be found using Table X. Table X will give the minimum interval length. $r = n-1 = 8$. $a = 2.623$, and $b = 21.595$. So, substituting in values into the above equation yields,

$$\left[\sqrt{\frac{27.63}{21.595}}, \sqrt{\frac{27.63}{2.623}}\right] = [1.131, 3.246].$$

(c) Find a 90% confidence interval for σ. Again Table X will be used to find the minimum interval length. $a = 3.298$ and $b = 19.110$. Thus,

$$\left[\sqrt{\frac{27.63}{19.110}}, \sqrt{\frac{27.63}{3.298}}\right] = [1.202, 2.894].$$

6.3-5 Let $X_1, X_2, ..., X_n$ be a random sample from $N(\mu, \sigma^2)$, with known mean μ. Describe how you would construct a confidence interval for the unknown variance σ^2.
HINT: Use the fact that $\frac{\sum_{i=1}^{n}(X_i-\mu)^2}{\sigma^2}$ is $\chi^2(n)$.

$$1 - \alpha = P\left[\frac{(n-1)E(s^2)}{b} \leq \sigma^2 \leq \frac{(n-1)E(s^2)}{a}\right].$$

$$E(s^2) = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \mu)^2, \ a = \chi^2_{\frac{\alpha}{2}}(n), \ b = \chi^2_{1-\frac{\alpha}{2}}(n).$$

So,

$$1 - \alpha = P\left[\frac{\sum_{i=1}^{n}(X_i - \mu)^2}{\chi^2_{\frac{\alpha}{2}}(n)} \leq \sigma^2 \leq \frac{\sum_{i=1}^{n}(X_i - \mu)^2}{\chi^2_{1-\frac{\alpha}{2}}(n)}\right].$$

6.3-6 Let $X_1, X_2, ..., X_n$ be a random sample of size n from an exponential distribution with unknown mean of $\mu = \theta$.

(a) Show that the distribution of $W = \frac{2}{\theta}\sum_{i=1}^{n} X_i$ is $\chi^2(2n)$.

$$M(t) \sim \chi^2(2n) = \frac{1}{(1-2t)^{\frac{2n}{2}}} = \frac{1}{(1-2t)^n}.$$

Simplifying the function W yields,

$$\frac{2}{\theta}\sum_{i=1}^{n} X_i = \frac{2n\bar{X}}{\theta}.$$

The moment generating function of an Exponential distribution is,

$$M(t) = \frac{1}{1-\theta t}.$$

$$M(t) = \int_0^\infty e^{\frac{2tx}{\theta}} \frac{1}{\theta} e^{-\frac{x}{\theta}}\, dx = \frac{1}{(1-2^t)}.$$

(b) Use W to construct a $100(1-\alpha)\%$ confidence interval for θ. Adapting the information given in Part (a) yields,

$$\left(\frac{2n\bar{x}}{\theta}, \frac{2n\bar{x}}{\theta}\right)$$

But, θ is unknown. It is known that θ is Chi distributed. So,

$$\left(\frac{2n\bar{x}}{\chi^2_{\frac{\alpha}{2}}(2n)}, \frac{2n\bar{x}}{\chi^2_{1-\frac{\alpha}{2}}(2n)}\right).$$

(c) If $n = 7$ and $\bar{x} = 93.6$, give the endpoints for a 90% confidence interval for θ.

$$\left(\frac{2(7)(93.6)}{23.68}, \frac{2(7)(93.6)}{6.571}\right) = (55.338, 199.422).$$

6.3-11 Some nurses were interested in the effect of prenatal care on the birthweight of babies. Mothers were divided into two groups, and their babies' weights were compared. The birthweight in ounces of babies of mothers who had received 5 or fewer prenatal visits were

49	108	110	82	93	114	134
114	96	52	101	114	120	116

and the birthweights of babies of mothers who had received 6 or more prenatal visits were

133	108	93	119	119	98	106
87	153	116	129	97	110	131

Assuming that these are respectively independent observations of X and Y, which are $N(\mu_X, \sigma_X^2)$ and $N(\mu_Y, \sigma_Y^2)$, find a 95% confidence interval for

(a) $\frac{\sigma_X^2}{\sigma_Y^2}$. This problem is similar to Example 6.3-3 in the text book.

$$\bar{x} = \frac{1}{14}\sum_{i=1}^{14} x_i = \frac{1403}{14} = 100.214,\ \bar{y} = \frac{1}{14}\sum_{i=1}^{14} y_i = \frac{1599}{14} = 114.214.$$

$$s_x^2 = \frac{1}{13}\sum_{i=1}^{14}(x_i - \bar{x})^2 = \frac{7858.3571}{13} = 604.489,\ s_y^2 = \frac{1}{13}\sum_{i=1}^{14}(y_i - \bar{x})^2 = \frac{4280.357144}{13} = 329.258.$$

The confidence interval is given by the following equation:

$$\left[c\frac{s_x^2}{s_y^2}, d\frac{s_x^2}{s_y^2}\right].$$

$$c = \frac{1}{F_{\frac{\alpha}{2},(n-1,m-1)}} = \frac{1}{3.115},\ d = F_{\frac{\alpha}{2},(m-1,n-1)} = 3.115.$$

Thus, the confidence interval is

$$\left[\frac{1}{3.115}\left(\frac{604.489}{329.258}\right), 3.115\left(\frac{604.489}{329.258}\right)\right] = [0.5894, 5.7489].$$

The above interval does not match the text book answer because it appears that the author used the statistic $F_{0.025,(12,12)} = 3.28$.

(b) $\frac{\sigma_X}{\sigma_Y}$. Taking square roots of the answer in (b) yields, $[0.7677, 2.3977]$

6.4-3 Let p equal the proportion of adult Americans who favor a law requiring a teenager to have her parents' consent before having an abortion. In a survey of 1000 adult Americans(conducted by *Times/*CNN and reported in *Time* on July 9, 1990), 690 said they favored such a law.

(a) Give a point estimate of p.

$$p = \frac{Y}{n} = \frac{690}{1000} = 0.690.$$

(b) Find an approximate 95% confidence interval of p. $z_{0.25} = 1.96$. The interval is given by the following equation:

$$\frac{Y}{n} \pm z_{0.25}\sqrt{\frac{\frac{Y}{n}\left(1 - \frac{Y}{n}\right)}{n}}.$$

$$0.690 \pm 1.96\sqrt{\frac{0.690(0.310)}{1000}} = 0.690 \pm 0.028666 = [0.6613, 0.7187].$$

6.4-7 In order to estimate the percentage of a large class of college freshmen that had high school GPAs from 3.2 to 3.5 inclusive, a sample of $n = 50$ students was taken, and $y = 9$ students fell in this class. Give a 95% confidence interval for the percentage of this freshman class having a high school GPA of 3.2 to 3.6. $p = \frac{Y}{n} = \frac{9}{50} = 0.18$. The confidence interval is given by, $p \pm 1.96\sqrt{\frac{0.18(0.82)}{50}} = [0.0735, 0.2865]$.

6.4-11 A candy manufacturer selects mints at random from the production line and weighs them. For one week, the day shift weighed $n_1 = 194$ mints, and the night shift weighed $n_2 = 162$ mints. The numbers of these mints that weighed at most 21 grams was $y_1 = 28$ for the day shift and $y_2 = 11$ for the night shift. Let p_1 and p_2 denote the proportions of mints that weigh at most 21 grams for the day and night shifts, respectively.

(a) Give a point estimate of p_1.

$$p_1 = \frac{y_1}{n_1} = \frac{28}{194} = 0.1443.$$

(b) Give the endpoints for a 95% confidence interval for p_1.

$$p_1 \pm z_{0.025}\sqrt{\frac{p_1 q_1}{n_1}} = 0.143 \pm 1.96\sqrt{\frac{(0.1443)(0.8557)}{194}} = [0.0949, 0.1937].$$

(c) Give a point estimate of $p_1 - p_2$. Solve for p_2 first.

$$p_2 = \frac{y_2}{n_2} = \frac{11}{162} = 0.0679.$$

$$p_1 - p_2 = 0.1443 - 0.0679 = 0.0764.$$

(d) Give the endpoints for a 95% confidence interval for $p_1 - p_2$.

$$p_1 - p_2 \pm z_{0.025}\sqrt{\frac{p_1 q_1}{n_1} + \frac{p_2 q_2}{n_2}} = 0.0764 \pm 1.96\sqrt{\frac{(0.1443)(0.8557)}{194} + \frac{(0.0679)(0.9321)}{162}} =$$

$$0.0764 \pm 0.0628 = [0.0136, 0.1392].$$

6.4-14 The following question was asked in a *Newsweek* poll: "Would you prefer to live in a neighborhood with mostly whites, with mostly blacks, or in a neighborhood mixed half and half?" Let p_1 and p_2 equal the proportion of black and white adult respondents, respectively, who prefer "half and half." If 207 out of 305 black adults and 291 out of 632 white adults prefer "half and half,"

(a) Give a point estimate of $p_1 - p_2$.

$$p_1 = \frac{Y_1}{n_1} = \frac{207}{305} = 0.6787,\ p_2 = \frac{Y_2}{n_2} = \frac{291}{632} = 0.4604.$$

$$p_1 - p_2 = 0.6787 - 0.4604 = 0.2183.$$

(b) Find an approximate 90% confidence interval for $p_1 - p_2$. $z_{\frac{\alpha}{2}} = 1.645$. The following equation will be used for the confidence interval,

$$p_1 - p_2 \pm z_{\frac{\alpha}{2}}\sqrt{\frac{p_1 q_1}{n_1} + \frac{p_2 q_2}{n_2}}.$$

So, substituting in the actual data yields,

$$0.2183 \pm 1.645\sqrt{\frac{(0.6787)(0.3213)}{305} + \frac{(0.4604)(0.5396)}{632}} = 0.2183 \pm 0.0548 = [0.1635, 0.2731]$$

6.4-15 An environmental survey contained a question asking what the respondent thought was the major cause of air pollution in this country, giving the choices "automobiles," "factories," and "incinerators." Two versions of the test, A and B, were used. Let p_A be the proportions of people using forms A and B who select "factories." If 170 out of 460 people who used version A chose "factories" and 141 out of 440 people who used version B chose "factories,"

(a) Find a 95% confidence interval for $p_A - p_B$. $n_A = 460$, $n_B = 440$, $y_A = 170$, and $y_B = 141$. Then,

$$p_A = \frac{y_A}{n_A} = \frac{170}{460} = 0.3696,\ p_B = \frac{y_B}{n_B} = \frac{141}{440} = 0.3205.$$

The confidence interval for $p_A - p_B$ is

$$0.3696 - 0.3205 \pm 1.96\sqrt{\frac{(0.3696)(0.6304)}{460} + \frac{(0.3205)(0.6795)}{440}} = 0.0491 \pm 0.062 =$$

$$[-0.0129, 0.111].$$

(b) Do the forms seem to be consistent concerning this answer? Why? Yes, the probability of one form A or B being biased cannot be accepted since zero is in the interval of the difference. Had one form or the other been biased, the confidence interval would have contained two negative numbers or two positive numbers.

6.5-2 Let X equal the excess weight of soap in a "1000-gram" bottle. Assume that the distribution of X is $N(\mu, 169)$. What sample size is required so that we have 95% confidence that the maximum error of the estimate of μ is 1.5? Note that $z_{\frac{\alpha}{2}} = 1.96$. The following equation will be used to determine the size of the sample: $z_{\frac{\alpha}{2}}\frac{\sigma}{\sqrt{n}} = error$. So,

$$1.96\left(\frac{\sqrt{169}}{\sqrt{n}}\right) = 1.5 \Rightarrow \sqrt{n} = \frac{1.96(\sqrt{169})}{1.5} \Rightarrow n = \left(\frac{1.96(\sqrt{169})}{1.5}\right)^2 \Rightarrow n = 288.55 \approx 289.$$

6.5-3 A company packages powered soap in "6-pound" boxes. The sample mean and standard deviation of the soap in these boxes are currently 6.09 and 0.02 pounds. If the mean fill can be lowered by 0.01 pounds, \$14,000 would be saved per year. Adjustments were made in the filling equipment.

(a) How large a sample is needed so that the maximum error of the estimate of the new μ is $\varepsilon = 0.001$ with 90% confidence? The sample size is calculated by solving for n in the following equation:

$$\varepsilon = \frac{z_{\frac{\alpha}{2}}\sigma}{\sqrt{n}}.$$

Substituting in actual values yields,

$$0.001 = \frac{1.645(0.02)}{\sqrt{n}} \Rightarrow \sqrt{n} = \frac{1.645(0.02)}{0.001} \Rightarrow n = \left(\frac{1.645(0.02)}{0.001}\right)^2 \Rightarrow n = 1082.41$$

Since n must be an integer set $n = 1083$.

(b) A random sample of size $n = 1219$ yielded $\bar{x} = 6.048$ and $s = 0.022$. Calculate a 90% confidence interval for μ. The following equation will be used to calculate the confidence interval:

$$\bar{x} \pm z_{\frac{\alpha}{2}}\frac{s}{\sqrt{n}}.$$

Substituting in actual data yields,

$$6.048 \pm 1.645\left(\frac{0.022}{\sqrt{1219}}\right) \Rightarrow 6.048 \pm 0.00104 = [6.047, 6.049].$$

(c) Estimate the savings per year with these new adjustments. The difference between the old mean and the new mean is $6.09 - 6.048 = 0.042$. It is given that \$14,000 is saved per 0.01 reduction in box weight. So, to find the savings in dollar amounts, $0.042\left(\frac{\$14{,}000}{0.01}\right) = \$58,800$.

(d) Estimate the proportion of boxes that will now weigh less than 6 pounds. In general, weight suggests a continuous random variable, not a discrete one. The question asks to find $P(\bar{X} < 6.0)$. Thus, the following integral will be used.

$$\int_0^6 \frac{x}{1219}\,dx = \left.\frac{x^2}{2(1219)}\right|_0^6 = \frac{36}{2(1219)} - 0 = 0.01477.$$

6.5-7 For a public opinion poll for a close presidential election, let p denote the proportion of voters who favor candidate A. How large a sample should be taken if we want the maximum error of the estimate of p to be equal to

(a) 0.03 with 95% confidence? Since p is unknown the following equation will have to be used:

$$n = \frac{z^2_{\frac{\alpha}{2}}}{4\varepsilon^2}$$

Substituting in actual data yields,

$$n = \frac{1.96^2}{4(0.03)^2} \Rightarrow n = 1067.111.$$

Setting n to the next integer, $n = 1068$.

(b) 0.02 with 95% confidence?

$$n = \frac{1.96^2}{4(0.02)^2} \Rightarrow n = 2401.$$

(c) 0.03 with 90% confidence?

$$n = \frac{1.645^2}{4(0.03)^2} \Rightarrow n = 751.7.$$

Setting n to the next integer, $n = 752$.

6.5-12 A seed distributor claims that 80% of its beet seeds will germinate. How many seeds must be tested for germination in order to estimate p, the true proportion that will germinate, so that the maximum error of the estimate is $\varepsilon = 0.03$ with 90% confidence? Since p is known, use the following equation,

$$z_{\frac{\alpha}{2}} \sqrt{\frac{\frac{Y}{n}\left(1 - \frac{Y}{n}\right)}{n}} = \varepsilon.$$

Substituting in actual values yields,

$$1.645\sqrt{\frac{(0.8)(0.2)}{n}} = 0.03 \Rightarrow \sqrt{\frac{(0.8)(0.2)}{n}} = \frac{0.03}{1.645} \Rightarrow \frac{(0.8)(0.2)}{n} = \left(\frac{0.03}{1.645}\right)^2 \Rightarrow$$

$$n = \frac{(0.8)(0.2)}{0.000332591} \Rightarrow n = 481.07.$$

Setting n to the next highest integer, $n = 482$.

7.4.5 Find the Power at Two Points

Fix the power at 2 points and find n and the constant c for the test.

Example: $X \sim N(\mu, \sigma^2)$, σ is known. $H_0 : \mu = \mu_0$ versus $H_1 : \mu > \mu_0$. Reject H_0 if $\bar{X} > c$. $K(\mu)$ is the power of the test. Fix $K(\mu_0 = \alpha)$ and $k(\mu)$ for one more given value of $\mu > \mu_0$. Let's take $\mu_0 = 50, K(50) = 0.05$, and $K(55) = 0.90$. $\sigma = 6$. Find n and c.

$$K(\mu) = P(\text{Reject } H_0|H_1) = P(\bar{X} > c|\mu) = P\left(\frac{\bar{X} - \mu}{\sigma/\sqrt{n}} > \frac{c - \mu}{\sigma/\sqrt{n}}\middle|\mu\right) = P\left(z > \frac{(c - \mu)\sqrt{n}}{\sigma}\middle|\mu\right) = K(\mu).$$

$$0.05 = K(50) = P\left(z > \frac{(c - 50)\sqrt{n}}{6}\right) \Rightarrow 0.05 = P(z > 1.645)$$

from the tables in the book. Then, $\frac{(c-50)\sqrt{n}}{6} = 1.645$. The second equation is derived as follow:

$$0.90 = P\left(z > \frac{(c-55)\sqrt{n}}{6}\right) \Rightarrow 0.90 = P(z > -1.282) \Rightarrow \frac{(c-55)\sqrt{n}}{6} = -1.282.$$

Solving both equations simultaneously yields $c = 52.8$ and $n = 12.42 \approx 13$.

Example: Problem 7.2-4 on page 410 of the test book. $Y \sim B(n,p)$. $H_0 : p = \frac{1}{2}$. versus $H_1 : p < \frac{1}{2}$. Reject H_0 if $y \leq c$. $K(p) = P\left(\text{Reject } H_0 | p < \frac{1}{2}\right)$. Assume large n.

$$P(y \leq c|p) = P\left(\frac{y-np}{\sqrt{pqn}} \leq \frac{c-np}{\sqrt{npq}}\right) = P\left(z \leq \frac{c-np}{\sqrt{npq}}\right) = K(p).$$

For $K(\frac{1}{2}) = 0.05$, and $K(\frac{1}{4}) = 0.90$, find n and c.

$$0.05 = P\left(z \leq \frac{c-n/2}{\sqrt{n/4}}\right) \Rightarrow 0.05 = P(z \leq -1.64) \Rightarrow \frac{c-n/2}{\sqrt{n/4}} = -1.64.$$

$$0.90 = P\left(z \leq \frac{c-n/4}{\sqrt{3n/16}}\right) \Rightarrow 0.90 = P(z \leq 1.282) \Rightarrow \frac{c-n/4}{\sqrt{3n/16}} = 1.282.$$

Solving both equations simultaneously yields $n = 30.4 \approx 31$ and $c = 10.8$. Reject H_0 if $y \leq 10.8$ which is the same as $y \leq 10$ due to discreteness.

$$\alpha = P\left(y \leq 10)|p = \frac{1}{2}\right) = P\left(y \leq 10.5|p = \frac{1}{2}\right) = P\left(z \leq \frac{10.5 - \frac{31}{2}}{4\sqrt{31}}\right) = 0.0362.$$

7.4.6 More on Hypothesis Testing

σ is known: $H_0 : \mu = \mu_0$. $H_1 : \mu > \mu_0$, or $H_1 : \mu < \mu_0$, or $H_1 : \mu \neq \mu_0$. The test statistic is $z = \frac{\bar{X}-\mu_0}{(\sigma/\sqrt{n})}$. $z \sim N(0,1)$.

σ is unknown: $H_0 : \mu = \mu_0$. $H_1 : \mu > \mu_0$. The test statistic is $T = \sqrt{n}\frac{(\bar{X}-\mu_0)}{S} \sim t(n-1)$. Note that $S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$.

H_1	Reject if:
$\mu > \mu_0$	$T > t_\alpha(n-1)$
$\mu < \mu_0$	$T < t_\alpha(n-1)$
$\mu \neq \mu_0$	$\lvert T\rvert > t_{\alpha/2}(n-1)$

Example: Problem 7.3-1 on page 416 of the text book. X is the growth of a tumor in 15 days. The hypotheses are as follow: $H_0 : \mu = \mu_0$. $H_1 : \mu \neq \mu_0$. $n = 9, \bar{X} = 4.3, S = 1.2, \alpha = 0.1$. $t_{0.05}(8) = 1.86$. The test statistic is $T = \frac{(4.3-4)\sqrt{9}}{1.2} = 0.75$. Since $0.75 < 1.86$, fail to reject H_0.

7.4.7 Testing About σ

$X \sim N(\mu, \sigma^2)$. Both μ and σ are unknown. $H_0 : \sigma = \sigma_0$.

H_1	Reject if:
$\sigma > \sigma_0$	$\chi^2 > \chi^2_\alpha(r)$
$\sigma < \sigma_0$	$\chi^2 < \chi^2_{1-\alpha}(r)$
$\sigma \neq \sigma_0$	$\chi^2 > \chi^2_{\alpha/2}$ or $\chi^2 < \chi^2_{1-\alpha/2}$

$$\frac{(n-1)S^2}{\sigma^2} \sim \chi^2(n-1),\ \frac{(n-1)S^2}{\sigma_0^2} \sim \chi^2(n-1).$$

The test statistic is $\chi^2 = \frac{(n-1)S^2}{\sigma_0^2}$. The power is given by

$$K(\sigma) = P(\text{Reject } H_0 : H_1) = P\left(\frac{(n-1)S^2}{\sigma^2} > \chi^2_\alpha(r) \middle| \sigma\right) = P\left(\frac{(n-1)S^2}{\sigma^2} > \frac{\sigma_0^2}{\sigma^2}\chi^2_\alpha(r)\right) =$$

$$P\left(\chi^2(n-1) > \frac{\sigma_0^2}{\sigma^2}\chi^2_\alpha(r)\right).$$

Example: A machine for filling tuna cans produces cans with a net weight having a $N(6.01, 0.0016)$. A new machine is available which claims to have a lower variability. Based on a sample of $n = 25$, $S^2 = 0.0009$, test at $\alpha = 0.05$, if the claim is justified. $H_0 : \sigma^2 = 0.0016$. $H_1 : \sigma^2 < 0.0016$. $\chi^2_{0.95}(24) = 13.85$. The test statistic is $\chi^2 = \frac{24(0.0009)}{0.0016} = 13.5$. Since $13.5 < 13.85$, reject H_0.

Suppose μ is known. Then use the following test statistic. $\sum_{i=1}^n \frac{(x_i-\mu)^2}{\sigma_0^2} \sim \chi^2(n)$. The degrees of freedom is different in the above expression.

7.4.8 Power of the Chi Square Test

Example: $X \sim N(\mu, \sigma^2)$. $H_0 : \mu = \mu_0$ versus $H_1 : \mu \neq \mu_0$. The confidence interval of μ is $\bar{X} \pm z_{\alpha/2}\frac{\sigma}{\sqrt{n}}$. The power of the Chi squared test is $H_0 : \sigma = \sigma_0$ versus $H_1 : \sigma = \sigma_1 > \sigma_0$. The test statistic is $\frac{(n-1)S^2}{\sigma_0^2} \sim \chi^2(n-1)$, if H_0 is true. Reject H_0 if $\chi^2 > \chi^2(n-1)$.

$$K(\sigma_1) = P(\text{Reject } H_0|H_1) = P\left(\frac{(n-1)S^2}{\sigma_0^2} > \chi^2_\alpha(n-1) \middle| H_1\right) = P\left(\frac{(n-1)S^2}{\sigma_1^2} > \frac{\sigma_0^2}{\sigma_1^2}\chi^2_\alpha(n-1) \middle| H_1\right) =$$

$$P\left(\chi^2_r > \frac{\sigma_0^2}{\sigma_1^2}\chi^2(r)\right) \geq \alpha.$$

Remember, the power is how often we reject H_0 correctly.

7.4.9 Power of Two Normals

$$X \sim N(\mu_x, \sigma_x^2),\ Y \sim N(\mu_y, \sigma_y^2).$$

Assume that $\sigma_x = \sigma_y = \sigma$, but are unknown. The hypothesis test is as follow: $H_0 : \mu_x = \mu_y$.

H_1	Reject if
$\mu_x > \mu_y$	$T > t_\alpha(r)$
$\mu_x < \mu_y$	$T < t_\alpha(r)$
$\mu_x \neq \mu_y$	$\lvert T\rvert > t_{\alpha/2}(r)$

$$\frac{\bar{X} - \bar{Y} - (\mu_x - \mu_y)}{S_p\sqrt{\frac{1}{n} + \frac{1}{m}}} \sim t(r), r = n + m - 2,\ S_p^2 = \frac{(n-1)S_x^2 + (m-1)S_y^2}{n+m-2}.$$

Under H_0, $\frac{\bar{X}-\bar{Y}}{S_p\sqrt{\frac{1}{n}+\frac{1}{m}}}$.

Example: Problem 7.4-1 on page 428 of the text book. Effect of 2 levels of hormones on pea steam. $n = 11, \bar{X} = 1.03, S_x^2 = 0.24$. $m = 13, \bar{Y} = 1.66, S_y^2 = 0.35$. $H_0 : \mu_x = \mu_y$. $H_1 : \mu_x < \mu_y$. $S_p^2 = \frac{(10)(0.24)+(12)(0.35)}{22} = 0.3 \Rightarrow S_p = 0.548$. $T = \frac{1.03-1.66}{0.548\sqrt{\frac{1}{11}+\frac{1}{13}}} = -2.81$. We reject H_0. We also assumed that $\sigma_x = \sigma_y$.

Suppose that $\sigma_x \neq \sigma_y$.

1. σ_x, σ_y are known. The test statistic is
$$z = \frac{\bar{X} - \bar{Y}}{\sqrt{\frac{\sigma_x^2}{n} + \frac{\sigma_y^2}{m}}} \sim N(0, 1).$$

2. σ_x, σ_y are unknown, but n, m are large. The test statistic is
$$z = \frac{\bar{X} - \bar{Y}}{\sqrt{\frac{S_x^2}{n} + \frac{S_y^2}{m}}} \approx N(0, 1).$$

3. σ_x, σ_y are unknown and n, m are small. The test statistic is
$$T = \frac{\bar{X} - \bar{Y}}{\sqrt{\frac{S_x^2}{n} + \frac{S_y^2}{m}}} \sim t(r),\ r = \frac{\left(\frac{S_x^2}{n} + \frac{S_y^2}{m}\right)^2}{\frac{1}{n-1}\left(\frac{S_x^2}{n}\right)^2 + \frac{1}{m-1}\left(\frac{S_y^2}{m}\right)^2}.$$

For the test for $\sigma_x = \sigma_y$, where X, Y are Normally distributed. $H_0 : \sigma_x = \sigma_y$.

H_1	Reject if
$\sigma_x > \sigma_y$	$F > F_\alpha(r_1, r_2)$
$\sigma_x < \sigma_y$	$F < F_{1-\alpha}(r_1, r_2)$
$\sigma_x \neq \sigma_y$	$F < F_{1-\alpha/2}(r_1, r_2)$ or $F > F_{\alpha/2}(r_1, r_2)$

$$F = \frac{S_x^2}{S_y^2} \sim F(r_1, r_2).$$

Example: Use the numbers in the previous example. $H_0 : \sigma_x = \sigma_y$ versus $H_1 : \sigma_x \neq \sigma_y$. $\alpha = 0.05$, $F = \frac{0.24}{0.35} = 0.686$, $r_1 = 10, r_2 = 12, \alpha/2 = 0.025$, $f_{0.025}(10, 12) = 3.37$, $f_{0.975}(10, 12) = \frac{1}{3.62} = 0.276$. Accept H_0.

7.4.10 Homework and Answers

6.6-4 Let $X_1, X_2, ..., X_n$ be a random sample from distributions with the following probability density functions. In each case find the maximum likelihood estimator $\hat{\theta}$.

(a) $f(x; \theta) = (1/\theta^2)xe^{-x/\theta}, 0 < x < \infty, 0 < \theta < \infty$.

$$L(\theta|x) = \prod_{i=1}^{n} \frac{1}{\theta^2} x_i e^{-\frac{x_i}{\theta}} \Rightarrow L(\theta|x) = \frac{1}{\theta^{2n}} e^{-\frac{\sum_{i=1}^n x_i}{\theta}} \prod_{i=1}^{n} x_i \Rightarrow L(\theta|x) = \frac{1}{\theta^{2n}} e^{-\frac{n\bar{X}}{\theta}} \prod_{i=1}^{n} x_i.$$

$$\log L(\theta|x) = \log 1 - \log \theta^{2n} - \frac{n\bar{X}}{\theta} + \log \prod_{i=1}^{n} x_i \Rightarrow \log L(\theta|x) = -2n \log \theta - \frac{n\bar{X}}{\theta} + \log \prod_{i=1}^{n} x_i$$

$$\frac{\partial \log L(\theta|x)}{\partial \theta} = \frac{-2n}{\theta} + \frac{n\bar{X}}{\theta^2} = 0 \Rightarrow -2n\theta = -n\bar{X} \Rightarrow \theta = \frac{\bar{X}}{2}.$$

Set $\hat{\theta} = \frac{\bar{X}}{2}$.

(b) $f(x;\theta) = (1/2\theta^3)x^2e^{-x/\theta}, 0 < x < \infty, 0 < \theta < \infty.$

$$L(\theta|x) = \prod_{i=1}^{n} \frac{1}{2}\theta^3 x_i^2 e^{-\frac{x_i}{\theta}} \Rightarrow L(\theta|x) = \frac{1}{2^n}\theta^{3n}e^{-\frac{\sum_{i=1}^{n} x_i}{\theta}} \prod_{i=1}^{n} x_i^2 \Rightarrow L(\theta|x) = \frac{\theta^{3n}}{2^n}e^{-\frac{n\bar{X}}{\theta}} \prod_{i=1}^{n} x_i^2.$$

$$\log L(\theta|x) = 3n\log\theta - n\log 2 - \frac{n\bar{X}}{\theta} + \log\prod_{i=1}^{n} x_i^2.$$

$$\frac{\partial \log l(\theta|x)}{\partial \theta} = \frac{3n}{\theta} + \frac{n\bar{X}}{\theta^2} = 0 \Rightarrow 3n\theta + n\bar{X} = 0 \Rightarrow 3n\theta = -n\bar{X} \Rightarrow \theta = -\frac{\bar{X}}{3}.$$

(c) $f(x;\theta) = (1/2)e^{-|x-\theta|}, -\infty < x < \infty, -\infty < \theta < \infty.$

$$L(\theta|x) = \prod_{i=1}^{n} \frac{1}{2}e^{-|x_i-\theta|} \Rightarrow L(\theta|x) = \frac{1}{2^n}e^{-|\sum_{i=1}^{n} x_i - n\theta|} \Rightarrow L(\theta|x) = \frac{1}{2^n}e^{-|n\bar{X}-n\theta|}.$$

$$\log L(\theta|x) = \log 1 - n\log 2 - n|\bar{X} - \theta|.$$

$\hat{\theta}$ is minimized at the sample median.

6.6-6 Let $f(x;\theta) = \theta x^{\theta-1}, 0 < x < 1, \theta \in \Omega = \theta : 0 < \theta < \infty$. Let $X_1, X_2, ..., X_n$ denote a random sample of size n from this distribution.

(a) Sketch the p.d.f. of X for (i) $\theta = 1/2$, (ii) $\theta = 1$, and (iii) $\theta = 2$. The graphs appear in the insert on the next page.

(b) Show that $\hat{\theta} = -n/\ln\prod_{i=1}^{n} X_i$ is the maximum likelihood estimator of θ.

$$L(\theta|x) = \prod_{i=1}^{n} \theta x_i^{\theta-1} \Rightarrow L(\theta|x) = \theta^n \prod_{i=1}^{n} x_i^{\theta-1}.$$

$$\log L(\theta|x) = n\log\theta + \log\prod_{i=1}^{n} x_i^{\theta-1} \Rightarrow \log L(\theta|x) = n\log\theta + (\theta-1)\log\prod_{i=1}^{n} x_i.$$

$$\frac{\partial \log L(\theta|x)}{\partial \theta} = \frac{n}{\theta} + \log\prod_{i=1}^{n} x_i = 0 \Rightarrow \theta\log\prod_{i=1}^{n} x_i = -n \Rightarrow \hat{\theta} = \frac{-n}{\log\prod_{i=1}^{n} x_i}.$$

(c) For each of the following three sets of 10 observations, calculate the maximum likelihood estimate(note that in Exercise 6.1-9 you were asked to find the method of moments estimates for θ) :

(i)	0.0256	0.3051	0.0278	0.8971	0.0739
	0.3191	0.7379	0.3671	0.9763	0.0102
(ii)	0.9960	0.3125	0.4374	0.7464	0.8278
	0.9518	0.9924	0.7112	0.2228	0.8609
(iii)	0.4698	0.3675	0.5991	0.9513	0.6049
	0.9917	0.1551	0.0710	0.2110	0.2154

For set (i):

$$\hat{\theta} = \frac{-n}{\log\prod_{i=1}^{n} x_i} = \frac{-10}{\ln 0.000000012} = 0.549.$$

For set (ii):

$$\hat{\theta} = \frac{-n}{\log \prod_{i=1}^{n} x_i} = \frac{-10}{\ln 0.010838702} = 2.21.$$

For set (iii):

$$\hat{\theta} = \frac{-n}{\log \prod_{i=1}^{n} x_i} = \frac{-10}{\ln 0.000029542} = 0.9588.$$

(d) Sketch the empirical and theoretic distribution functions (using $\hat{\theta}$ as the value of the parameter) on the same graph for each set of data. Comment on the fit. For the graphs, look on one of the following pages. As theta increases, the curve seems to bow downward more and more.

6.6-7 Out of 50,000,000 instant winner lottery tickets, the proportion of winning tickets is p. Each day, for 20 consecutive days, a bettor purchased tickets, one at a time, until a winning ticket was purchased. The numbers of tickets that were purchased each day to obtain the winning ticket were

1	26	19	6	6	1	2	3	1	23
19	3	6	8	4	1	18	34	1	8

By making reasonable assumptions, find the maximum likelihood estimate of p based on these data. Waiting for the first Bernoulli success suggests the Geometric distribution. So the p.d.f. is $f(x) = (1-p)^{x-1}p$.

$$L(p|x) = \prod_{i=1}^{n} p(1-p)^{x_i - 1} \Rightarrow L(p|x) = p^n (1-p)^{\sum_{i=1}^{n} x_i - n} \Rightarrow L(p|x) = p^n (1-p)^{n(\bar{X}-1)}.$$

$$\log L(p|x) = n \log p + (n(\bar{X}-1)) \log(1-p).$$

$$\frac{\partial \log L(p|x)}{\partial p} = \frac{n}{p} - \frac{n(\bar{X}-1)}{1-p} = 0 \Rightarrow \frac{1-p}{p} - \bar{X} + 1 = 0 \Rightarrow \frac{1}{p} - \bar{X} = 0 \Rightarrow p = \frac{1}{\bar{X}}.$$

Solving for $\bar{X}$,

$$\bar{X} = \frac{1}{20} \sum_{i=1}^{20} x_i = \frac{190}{20} = 9.5.$$

So, substituting in the value of $\bar{X}$ yields, $p = \frac{1}{9.5} = 0.10526$.

6.7-1 Let $X_1, X_2, ..., X_n$ be a random sample of size n from the exponential distribution whose p.d.f. is $f(x;\theta) = (1/\theta)e^{-x/\theta}, 0 < x < \infty, 0 < \theta < \infty$. We know that $\bar{X}$ is an unbiased estimator for θ and the variance of $\bar{X}$ is θ^2/n so that $\bar{X}$ is the best unbiased estimator for θ.

$$\log f(x;\theta) = \log 1 - \log \theta - \frac{x}{\theta}, \quad \frac{\partial \log f(x;\theta)}{\partial \theta} = -\frac{1}{\theta} + \frac{x}{\theta^2}, \quad \frac{\partial^2 \log f(x;\theta)}{\partial \theta^2} = \frac{1}{\theta^2} - \frac{2x}{\theta^3}.$$

$$E\left(-\frac{\partial^2 \log f(x;\theta)}{\partial \theta^2}\right) = \frac{2E(x)}{\theta^3} - \frac{1}{\theta^2} = \frac{2\theta}{\theta^3} - \frac{1}{\theta^2} = \frac{2}{\theta^2} - \frac{1}{\theta^2} = \frac{1}{\theta^2} = I(\theta).$$

The lower bound is given by the following equation: $\frac{1}{nI(\theta)} = \frac{\theta^2}{n}$.

6.7-3 Let $X_1, X_2, ..., X_n$ denote a random sample from $b(1, p)$. We know that $\bar{X}$ is an unbiased estimator of p and that $Var(\bar{X}) = p(1-p)/n$. (See Exercise 6.1-3).

(a) Find the Rao-Cramer lower bound for $\bar{X}$.

$$\log f(n, p) = \log 1 - \log x!(1-x)! + x \log p + (1-x)\log(1-p).$$

$$\frac{\partial \log f(n,p)}{\partial p} = \frac{x}{p} - \frac{1-x}{1-p}, \quad \frac{\partial^2 \log f(n,p)}{\partial p^2} = -\frac{x}{p^2} - \frac{1-x}{(1-p)^2}.$$

$$E\left(-\frac{\partial^2 \log f(n,p)}{\partial p^2}\right) = \frac{E(x)}{p^2} + \frac{1-E(x)}{(1-p)^2} = \frac{p}{p^2} + \frac{1-p}{(1-p)^2} = \frac{1}{p} + \frac{1}{p-1} = \frac{(1-p)+p}{p(1-p)} =$$

$$\frac{1}{p(1-p)} = I(p).$$

The lower bound is given by the following equation, $\frac{1}{nI(p)} = \frac{p(1-p)}{n}$.

(b) What is the efficiency of $\bar{X}$ as an estimator of p? The efficiency of an estimator is the ratio of the Rao-Cramer lower bound and the estimator. So,

$$\frac{\frac{p(1-p)}{n}}{\frac{p(1-p)}{n}} 100\% = 100\%.$$

7.1-1 Bowl A contains 100 red balls and 200 white balls; bowl B contains 200 red balls and 100 white balls. Let p denote the probability of drawing a red ball from a bowl, but say p is unknown, since it is unknown whether bowl A or bowl B is being used. We shall test the simple null hypothesis $H_0 : p = 1/3$ against the simple alternative hypothesis $H_1 : p = 2/3$. Draw three balls at random, one at a time and with replacement from the selected bowl. Let X equal the number of red balls drawn. Then let the critical region be $C = x : x = 2, 3$. What are the values of α and β, the probabilities of Type I and Type II errors, respectively? Solve for α first.

$$\alpha = P(x = 2, x = 3|p = 1/3) = \sum_{x=2}^{3} \left(\begin{array}{c} 3 \\ x \end{array} \right) \left(\frac{1}{3}\right)^x \left(\frac{2}{3}\right)^{3-x} \Rightarrow \alpha = 3\left(\frac{1}{3}\right)^2 \left(\frac{2}{3}\right) + \left(\frac{1}{3}\right)^3 \Rightarrow$$

$$\alpha = \frac{3}{9}\left(\frac{2}{3}\right) + \frac{1}{27} = \frac{7}{27}.$$

Next, solve for β.

$$\beta = P(x \neq 2, 3|p = 2/3) = 1 - P(x = 2, 3|p = 2/3).$$

$$\beta = 1 - \sum_{x=2}^{3} \left(\begin{array}{c} 3 \\ x \end{array} \right) \left(\frac{2}{3}\right)^x \left(\frac{1}{3}\right)^{3-x} \Rightarrow \beta = 1 - 3\left(\frac{2}{3}\right)^2 \left(\frac{1}{3}\right) - \left(\frac{2}{3}\right)^3 = 1 - \frac{12}{27} - \frac{8}{27} \Rightarrow \beta = \frac{7}{27}.$$

7.1-4 Let p denote the probability that, for a particular tennis player, the first serve is good. Since $p = 0.40$, this player decided to take lessons in order to increase p. When the lessons are completed, the hypothesis $H_0 : p = 0.40$ will be tested against $H_1 : p > 0.40$ based on $n = 25$ trials. Let y equal the number of first serves that are good, and let the critical region be defined by $C = y : y \geq 13$.

(a) Determine $\alpha = P(Y \geq 13; p = 0.40)$. Use Table II in the Appendix.

$$\alpha = P(Y \geq 13|p = 0.40) = 1 - P(Y \leq 12|p = 0.40) = 1 - 0.8462 = 0.1538.$$

(b) Find $\beta = P(Y < 13)$ when $p = 0.60$; that is, $\beta = P(Y \leq 12; p = 0.60)$. Use Table II.

7.1-7 If a newborn baby has a birth weight that is less than 2500 grams(5.5 pounds), we say that the baby has a low birth weight. The proportion of babies with a low birth weight is an indicator of nutrition (or lack of nutrition) for the mothers. For the United States, approximately 7% of babies have a low birth weight. Let p equal the proportion of babies born in the Sudan who weigh less than 2500 grams. We shall test the null hypothesis $H_0 : p = 0.07$ against the alternative hypothesis $H_1 : p > 0.07$. If $y = 23$ babies out of a random sample of $n = 209$ babies weighed less than 2500 grams, what is your conclusion at a significance level of

(a) $\alpha = 0.05$? The null hypothesis will be rejected if the following inequality holds true:

$$z = \frac{\frac{23}{209} - 0.07}{\sqrt{\frac{(0.07)(0.93)}{209}}} \geq z_{0.05}$$

$z_{0.05} = 1.645$ Since $2.269 > 1.645$, the null hypothesis is rejected. More than 7% of the babies in the Sudan have low birth weights.

(b) $\alpha = 0.01$? The null hypothesis will be rejected if the following inequality holds true:

$$z = \frac{\frac{23}{209} - 0.07}{\sqrt{\frac{(0.07)(0.93)}{209}}} \geq z_{0.01}$$

$z_{0.01} = 2.326$. Since $2.269 < 2.326$, the null hypothesis is accepted. 7% of the babies in the Sudan have low birth weights.

7.1-10 Let p equal the proportion of drivers who use a seat belt in a state that does not have a mandatory seat belt law. It was claimed that $p = 0.14$. An advertising campaign was conducted to increase this proportion. Two months after the campaign, $y = 104$ out of a random sample of $n = 590$ drivers were wearing their seat belts. Was the campaign successful?

(a) Define the null and alternative hypotheses. $H_0 : p = 0.14$ versus $H_1 : p > 0.14$.

(b) Define a critical region with an $\alpha = 0.01$ significance level.

$$z = \frac{\frac{Y}{n} - p_0}{\sqrt{\frac{(p_0)(1-p_0)}{n}}} \geq z_\alpha.$$

(c) What is your conclusion?

$$z = \frac{\frac{104}{590} - 0.14}{\sqrt{\frac{(0.14)(0.86)}{590}}} \geq 2.326.$$

Since $2.539 \geq 2.326$, the null hypothesis is rejected. The campaign increased the number of people who wear seat belts.

7.1-16 A machine shop that manufactures toggle levers has both a day and a night shift. A toggle lever is defective if a standard nut cannot be screwed onto the threads. Let p_1 and p_2 be the proportion of defective levers among those manufactured by the day and night shifts, respectively. We shall test the null hypothesis, $H_0 : p_1 = p_2$, against a two-sided alternative hypothesis based on two random samples, each of 1000 levers taken from the production of the respective shifts.

(a) Define the test statistic and a critical region that has an $\alpha = 0.05$ significance level. Sketch a standard normal p.d.f. illustrating this critical region.

(b) If $y_1 = 37$ and $y_2 = 53$ defectives were observed for the day and night shifts, respectively, calculate the value of the test statistic. Locate the calculated test statistic on your figure in part (a) and state your conclusion. First solve for $\hat{p}, \hat{p}_1, \hat{p}_2$.

$$\hat{p} = \frac{y_1 + y_2}{n_1 + n_2} = \frac{37 + 53}{2000} = 0.045,\ \hat{p}_1 = \frac{37}{1000} = 0.037,\ \hat{p}_2 = \frac{53}{1000} = 0.053.$$

Substituting in values into the above inequality yields,

$$\frac{|0.037 - 0.053|}{\sqrt{\frac{(0.045)(0.955)}{2000}}} \geq 1.96.$$

Since $3.452 \geq 1.96$, the null hypothesis is rejected. The defective rate of levers among the day and night shift is different.

7.2-1 A certain size bag is designed to hold 25 pounds of potatoes. A farmer fills such bags in the field. Assume that the weight X of potatoes in a bag is $N(\mu, 9)$. We shall test the null hypothesis $H_0 : \mu = 25$ against the alternative hypothesis $H_1 : \mu < 25$. Let x_1, X_2, X_3, X_4 be a random sample of size 4 from this distribution, and let the critical region C for this test be defined by $\bar{x} \leq 22.5$, where $\bar{x}$ is the observed value of $\bar{X}$.

(a) What is the power function $K(\mu)$ for this test? In particular, what is the significance level $\alpha = K(25)$ for your test?

$$K(\mu) = P(\bar{X} \leq 22.5; \mu) = P\left(\frac{\bar{X} - \mu}{\sigma/\sqrt{n}} \leq \frac{22.5 - \mu}{\sigma\sqrt{n}}; \mu\right).$$

Specifically, for $K(25)$,

$$\alpha = \Phi\left(\frac{22.5 - 25}{3/2}\right) = \Phi(-1.67) = 0.0475.$$

(b) If the random sample of four bags of potatoes yielded the values $x_1 = 21.24, x_2 = 24.81, x_3 = 23.62, x_4 = 26.82$, would you accept or reject H_0 using your test?

$$\bar{x} = \frac{1}{4}\sum_{i=1}^{4} x_i = \frac{96.49}{4} = 24.1225.$$

Since $24.1225 > 22.5$, fail to reject H_0.

(c) What is the p-value associated with the $\bar{x}$ in part (b)?

$$\Phi\left(\frac{24.1225 - 25}{3/2}\right) = \Phi(-0.59) = 0.2776.$$

7.2-5 Let X equal the yield of alfalfa in tons per acre per year. Assume that X is $N(1.5, 0.09)$. It is hoped that new fertilizer will increase the average yield. We shall test the null hypothesis $H_0 : \mu = 1.5$ against the alternative hypothesis $H_1 : \mu > 1.5$. Assume that the variance continues to equal $\sigma^2 = 0.09$ with the new fertilizer. Using $\bar{X}$, the mean of a random sample of size n, as the test statistic, reject H_0 if $\bar{x} \geq c$. Find n and c so that the power function $K(\mu) = P(\bar{X} \geq c : \mu$ is such that $\alpha = K(1.5) = 0.05$ and $K(1.7) = 0.95$.

$$K(\mu) = P(\text{Reject } H_0|H_1) = P(\bar{X} > c|\mu) = P\left(\frac{\bar{X} - \mu}{\sigma/\sqrt{n}} > \frac{c - \mu}{\sigma/\sqrt{n}}\right) = P\left(z > \frac{(c - \mu)\sqrt{n}}{\sigma}\right).$$

For $\alpha = K(1.5) = 0.05$,

$$P\left(z > \frac{(c-1.5)\sqrt{n}}{\sigma}\right) = 0.05 \Rightarrow z = 1.645.$$

That leads to the following equation:

$$\frac{(c-1.5)\sqrt{n}}{\sqrt{0.09}} = 1.645. \tag{7.1}$$

Now, to find the second equation,

$$0.95 = P\left(z > \frac{(c-1.7)\sqrt{n}}{\sigma}\right) \Rightarrow z = -1.645.$$

So,

$$\frac{(c-1.7)\sqrt{n}}{\sqrt{0.09}} = -1.645. \tag{7.2}$$

Solving equations 7.1 and 7.2 simultaneously yields, $n = 24.354 \approx 25$. $c = 1.6$.

7.2-9 Let p denote the probability that, for a particular tennis player, the first serve is good. Since $p = 0.40$, this player decided to take lessons in order to increase p. When the lessons are completed, the hypothesis $H_0 : p - 0.40$ will be tested against $H_1 : p > 0.40$ based on $n = 25$ trials. Let y equal the number of first serves that are good, and let the critical region be defined by $C = y : y \geq 14$.

(a) Define the power function $K(p)$ for this test. The exact value of $K(p)$ is given by,

$$K(p) = \sum_{y=14}^{25} \binom{25}{y} (0.40)^y (0.60)^{25-y},$$

(b) What is the value of the significance level, $\alpha = K(0.40)$? Use Appendix Table II.

$$K(p) = P(Y \geq 14|p) = P\left(\frac{Y-np}{\sqrt{npq}} \geq \frac{c-np}{\sqrt{npq}}\right).$$

For $\alpha = K(0.40)$,

$$P\left(z \geq \frac{c - 25(0.40)}{\sqrt{25(0.40)(0.60)}}\right) = 1 - P\left(z < \frac{c-10}{2.4495}\right) = 1 - 0.9222 = 0.0778.$$

(c) Evaluate $K(p)$ at $p = 0.45, 0.50, 0.60, 0.70, 0.80$, and 0.90. Use Table II.

For $K(0.45)$, $1 - 0.8173 = 0.1827$.
For $K(0.50)$, $1 - 0.655 = 0.345$.
For $K(0.60)$, re-solve for y since $p > 0.50$. $y = 25 - 14 = 11$. So, $K(0.60) = 0.7323$.
For $K(0.70)$, 0.9558.
For $K(0.80)$, 0.9985.
For $K(0.90)$, 1.0.

(d) Sketch the graph of the power function. See the insert on the next page for the graph.

(e) If $y = 15$ first serves were good following the lessons, would H_0 be rejected? Yes, since $y = 15 > 14$.

(f) What is the p-value associated with $y = 15$?

$$K(p) = \sum_{y=15}^{25} \binom{25}{y} (0.40)^y (0.60)^{25-y} \Rightarrow K(p) = 1 - \sum_{y=1}^{14} \binom{25}{y} (0.40)^y (0.60)^{25-y} = 0.0344.$$

7.2-12 Let X_1, X_2, X_3 be a random sample of size $n = 3$ from an exponential distribution with mean $\theta > 0$. Reject the simple null hypothesis $H_0 : \theta = 2$ and accept the composite alternative hypothesis $H_1 : \theta < 2$ if the observed sum $\sum_{i=1}^{3} x_i \leq 2$.

(a) What is the power function $K(\theta)$ written as an integral?

$$T = \sum_{i=1}^{3} x_i \sim Gamma(3, \theta).$$

The critical region is given by:

$$H_0 : P(T < 2|\theta < 2) = \int \frac{e^{-\frac{t}{\theta}} t^{3-1}}{\Gamma(3)\theta^3}\, dt.$$

(b) Using integration by parts, define the power function as a summation.

(c) With the help of Table III in the Appendix, determine $\alpha = K(2), K(1), K(1/2)$, and $K(1/4)$.

7.4.11 One-way ANOVA

Here are some examples of uses for a one-way ANOVA table:

1. Average miles per gallon for different car models.
2. Several different drugs for controlling blood pressure.

There are m different populations. $X_i \sim N(\mu, \sigma^2), i = 1, ..., m$. $H_0 : \mu_1 = \mu_2 = \cdots = \mu_m$. $H_1 : \mu_i \neq \mu_j, i, j \in 1, ..., m$. From the $i - th$ population, let $x_{ij}, i = 1, 2, ..., n_i$ be a random sample.

Mean	Variance	Population					
μ_1	σ^2	x_{11}	$\cdots$	x_{1j}	$\cdots$	x_{1n_1}	$\bar{X}_1$
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
μ_i	σ^2	x_{i1}	$\cdots$	x_{ij}	$\cdots$	x_{in_i}	$\bar{X}_i$
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
μ_m	σ^2	x_{m1}	$\cdots$	x_{mj}	$\cdots$	x_{mn_m}	$\bar{X}_m$

$n = \sum_{i=1}^{m} n_i$, where n_i is the sample size of the $i - th$ population.

$$\sum_{i=1}^{m}\sum_{j=1}^{n_i}(x_{ij} - \bar{X})^2,\ \bar{X}_{i\cdot} = \frac{1}{n_i}\sum_{j=1}^{n_i} x_{ij},\ \bar{X} = \frac{1}{n}\sum_{i=1}^{m}\sum_{j=1}^{n_i} x_{ij}.$$

$$\sum_{i=1}^{m}\sum_{j=1}^{n_i}(x_{ij} - \bar{X})^2 = \sum_{i=1}^{m}\sum_{j=1}^{n_i}(x_{ij} - \bar{X}_{i\cdot} + \bar{X}_{i\cdot} - \bar{X})^2 =$$

$$\sum_{i=1}^{m}\sum_{j=1}^{n_i}[(x_{ij} - \bar{X}_{i\cdot})^2 + (\bar{X}_{i\cdot} - \bar{X})^2 + 2(x_{ij} - \bar{X}_{i\cdot})(\bar{X}_{i\cdot} - \bar{X}).$$

The total sum of squares is

$$\sum_{i=1}^{m}\sum_{j=1}^{n_i}(x_{ij} - \bar{X}_{i\cdot})^2 + \sum_{i=1}^{m} n_i(\bar{X}_{i\cdot} - \bar{X})^2 + 0.$$

$SS(TOT) = SS(E) + SS(TRT)$. $SS(TRT)$ is the sum of squares due to treatments. $x_1, ..., x_n \sim N(\mu, \sigma^2)$,

$$\frac{1}{\sigma^2}\sum_{i=1}^{m}(x_i - \bar{X})^2 \sim \chi^2(n-1).$$

The distribution of $\sum(x_i - \bar{X})^2$ does not depend on μ.

$$\frac{1}{\sigma^2}\sum_{i=1}^{m}\sum_{j=1}^{n_i}(x_{ij} - \bar{X})^2 \sim \chi^2(n-m),\ \frac{1}{\sigma^2}\sum_{j=1}^{n_i}(x_{ij} - \bar{X}_{i\cdot})^2 \sim \chi^2(n_i - 1).$$

If H_0 is true then,

$$\frac{1}{\sigma^2}\sum_{i=1}^{m}\sum_{j=1}^{n_i}(x_{ij} - \bar{X})^2 \sim \chi^2(n-1).$$

Theorem: Reference page 459 of the text book. Let $Q = Q_1 + Q_2 + \cdots + Q_k$, where Q's are real quadratic forms in independent random variables Normally distributed with the same σ^2. Let $\frac{Q}{\sigma^2}, \frac{Q_1}{\sigma^2}, ..., \frac{Q_k}{\sigma^2}$ have a Chi squared distribution with $r, r_1, ..., r_k$ degrees of freedom. If $Q_k \geq 0$, then

1. $Q_1, ..., Q_k$ are mutually independent.
2. $\frac{Q_k}{\sigma^2} \sim \chi^2(r_k)$, where $r_k = r - (r_1 + ... + r_{k-1}) = r - \sum_{i=1}^{k-1} r_i$. So, $\frac{1}{\sigma^2}\sum_{i=1}^{m} n_i(x_{i\cdot} - \bar{X})^2 \sim \chi^2(m-1)$ only if H_0 is true.

$$E\left[\frac{\sum_{i=1}^{m}\sum_{j=1}^{n_i}(x_{ij} - \bar{X}_{i\cdot})^2}{\sigma^2}\right] = n - m \Rightarrow E\left[\frac{\sum_{i=1}^{m}\sum_{j=1}^{n_i}(x_{ij} - \bar{X}_{i\cdot})^2}{n-m}\right] = \sigma^2.$$

$$E\left[\sum_{i=1}^{m} n_i(\bar{X}_{i\cdot} - \bar{X})^2\right] = E\left[\sum_{i=1}^{m} n_i\bar{X}_{i\cdot}^2 - n\bar{X}^2\right] = \sum_{i=1}^{m} n_i E(\bar{X}_{i\cdot})^2 - nE(\bar{X})^2.$$

$$\bar{X}_{i\cdot} \sim N\left(\mu_i, \frac{\sigma^2}{n_i}\right),\ \bar{X} = \frac{1}{n}\sum_{i=1}^{m} n_i\bar{X}_{i\cdot} \sim N\left(\bar{\mu}, \frac{\sigma^2}{n}\right).$$

Thus,

$$(m-1)\sigma^2 + \sum_{i=1}^{m} n_i(\mu_i - \bar{\mu})^2 \text{ where } \bar{\mu} = \frac{1}{n}\sum_{i=1}^{m} n_i\mu_i.$$

Thus,

$$E\left[\frac{1}{m-1}\sum_{i=1}^{m} n_i(\bar{X}_{i\cdot} - \bar{X})^2\right] = \sigma^2\frac{1}{m-1}\sum_{i=1}^{m} n_i(\mu_i - \mu)^2.$$

If H_0 is true, then

$$E\left[\frac{1}{m-1}\sum_{i=1}^{m} n_i(\bar{X}_i - \bar{X})^2\right] = \sigma^2 + 0 = \sigma^2.$$

ANOVA Table

Source	SS	MS	df
Treatment	$\sum_{i=1}^{m} n_i(\bar{X}_{i\cdot} - \bar{X})^2$	$SS(TRT)/(m-1)$	$m-1$
Error	$\sum_{i=1}^{m}\sum_{j=1}^{n_i}(x_{ij} - \bar{X}_{i\cdot})^2$	$SS(E)/(n-m)$	$n-m$
Total	$\sum_{i=1}^{m}\sum_{j=1}^{n_i}(x_{ij} - X)^2$	$SS(TOT)/9n-1)$	$n-1$

The test statistic is

$$F = \frac{MS(TRT)}{MS(E)} \sim F(m-1, n-m).$$

Reject H_0 for large values of F. To simplify the calculations, use the following expressions:

$$T_i = \sum_{j=1}^{n_i} x_{ij} = \text{total of the i-th sample, } T = \sum_{i=1}^{m} T_i = \text{total of all n observations.}$$

$$\bar{X}_{i\cdot} = \frac{T_i}{n_i},\ \bar{X} = \frac{T}{n}.$$

The sum of squares of the total is given by,

$$\sum_{i=1}^{m}\sum_{j=1}^{n_i}(x_{ij} - \bar{X})^2 = \sum_{i=1}^{m}\sum_{j=1}^{n_i} x_{ij}^2 - n\bar{X}^2 = \sum_{i=1}^{m}\sum_{j=1}^{n_i} x_{ij}^2 - \frac{T^2}{n}.$$

$$SS(TOT) = \sum_{i=1}^{m} n_i(x_ij - \bar{X})^2 = \sum_{i=1}^{m} n_i\bar{X}_{i\cdot}^2 - n\bar{X}^2 = \sum_{i=1}^{m}\frac{T_i^2}{n_i} - \frac{T^2}{n}.$$

$SS(E) = SS(TOT) - SS(TRT)$.

Example: Problem 8.1-1 on page 460 of the text book. $m = 4, n_i = 3, i = 1, 2, 3, 4., n = 12$.

m				$\bar{X}_{i\cdot}$	μ_i
1	13	8	9	10	μ_1
2	15	11	13	13	μ_2
3	8	12	7	9	μ_3
4	11	15	10	12	μ_4

$H_0 : \mu_1 = \mu_2 = \mu_3 = \mu_4$.

Source	SS	df	MS	F	p-value
Treatment	30	3	10	1.6	0.264
Error	50	8	6.25		
Total	80	11			

Suppose, $\alpha = 0.05, r_1 = 3, r_2 = 8$. Then,$F_{0.05}(3, 8) = 4.07$. Thus, we accept H_0.

7.4.12 Two-way ANOVA

Involves an experiment with 2 treatments at different levels. Factor A has a different levels and Factor B has b different levels. x_{ij} is the observation for factor A at level i and factor B at level j.

	1	2	3	...	b	
1	x_{11}	X_{12}	x_{13}	...	X_{1b}	$\bar{X}_1$
2	x_{21}	X_{22}	x_{23}	...	X_{2b}	$\bar{X}_2$
.						
.						
.						
i	x_{i1}	X_{i2}	x_{i3}	...	X_{ib}	$\bar{X}_i$
.						
.						
.						
a	x_{a1}	X_{a2}	x_{a3}	...	X_{ab}	$\bar{X}_a$

$x_{ij} \sim N(\mu_i, \sigma^2)$. The model statement is as follow:

$$\mu_{ij} = \mu + \alpha_i + \beta_j + \epsilon_{ij},\ \sum_{i=1}^{a} \alpha_i = \sum_{j=1}^{b} \beta_j = 0,\ \epsilon_{ij} \sim N(0, \sigma^2).$$

α_i is the effect of the $i - th$ level of factor A. β_j is the effect of the $j - th$ level of factor B.

$$\bar{X}_{i\cdot} = \frac{1}{b} \sum_{j=1}^{b} x_{ij}.$$

$$\sum_{i=1}^{a} \sum_{j=1}^{b} (x_{ij} - \bar{X})^2 = b \sum_{i=1}^{a} (\bar{X}_{i\cdot} - \bar{X})^2 + a \sum_{j=1}^{b} (\bar{X}_{\cdot j} - \bar{X})^2 + \sum_{i=1}^{a} \sum_{j=1}^{b} (x_{ij} - \bar{X}_{i\cdot} - \bar{X}_{\cdot j} + \bar{X})^2.$$

$$\sum_{i=1}^{a} \sum j = 1^b (x_{ij} - \bar{X})^2 = \sum_{i=1}^{a} \sum_{j=1}^{b} (x_{ij} - \bar{X}_{i\cdot} - \bar{X}_{\cdot j} + \bar{X} + \bar{X}_{i\cdot} - \bar{X} + \bar{X}_{\cdot j} - \bar{X})^2.$$

$SS(TOT) = SS(A) + SS(B) + SS(E)$. Estimate μ, α_i, β_j by minimizing the following

$$\sum_{i=1}^{a} \sum_{j=1}^{b} (x_{ij} - \mu - \alpha_i - \beta_j)^2 = \sum_{i=1}^{a} \sum_{j=1}^{b} \epsilon_{ij}^2 = S^2,$$

$$\frac{\partial S}{\partial \mu} = 0 \Rightarrow \hat{\mu} = \bar{X},\ \frac{\partial S}{\partial \alpha_i} = 0 \Rightarrow \hat{\alpha}_i = \bar{X}_{i\cdot} - \bar{X},\ \frac{\partial S}{\partial \beta_j} = \bar{X}_{\cdot j} - \bar{X}.$$

ANOVA Table

Source	SS	df	MS
Factor A	$b \sum_{i=1}^{a} (X_{i\cdot} - X)^2$	$a - 1$	$SS(A)/(a-1)$
Factor B	$a \sum_{j=1}^{b} (\bar{X}_{\cdot j} - \bar{X})^2$	$b - 1$	$SS(B)/(b-1)$
Error	SS(E)	$(a-1)(b-1)$	$SS(E)/[(a-1)(b-1)]$
Total		ab-1	

$$E[MS(A)] = \sigma^2 + \frac{b}{a-1} \sum_{i=1}^{a} \alpha_i^2,\ E[MS(B)] = \sigma^2 + \frac{a}{b-1} \sum_{j=1}^{b} \beta_j^2,\ E[MS(E)] = \sigma^2.$$

$H_A : \alpha_1 = \alpha_2 = ... = \alpha_a = 0$, versus $H_B : \beta_1 = \beta_2 = ... = \beta_b = 0$. $\frac{MS(A)}{MS(E)} \sim F(a-1, r)$, $\frac{MS(B)}{MS(E)} \sim F(b-1, r)$.

Example: Problem 8.2-1 on page 471 of the text book. $a = 3$(different models of cars) and $b = 4$(different brands of gasoline).

Source	SS	df	MS	F
Cars	24	2	12	18
Gas	30	3	10	15
Error	4	6	$\frac{2}{3}$	
Total	58	11		

For $\alpha = 0.01, F_1 = 10.92, F_2 = 9.78$. $H_A : \alpha_1 = \alpha_2 = \alpha_3 = 0$, versus Reject H_A. $H_B : \beta_1 = \beta_2 = \beta_3 = \beta_4 = 0$. Reject H_B.

7.4.13 Two-way ANOVA with Replication

Treatments A at a levels and B at b levels. $x_{ijk}, k = 1, 2, ...c$ for the $i - th$ level of treatment A and the $j - th$ level of treatment B. The total number of observations is $n = abc$. The model statement is $x_{ijk} = \mu + \alpha_i + \beta_j + \gamma_{ij} + \epsilon_{ijk}$. Assume that

$$\sum_{i=1}^{a} \alpha_i = \sum_{j=1}^{b} \beta_j = \sum_{(A)} \gamma_{ij} = 0.$$

$$\sum_{ijk} (x_{ijk} - \bar{X})^2 =$$

$$\overbrace{bc\sum_{i=1}^{a}(\bar{X}_{i\cdot\cdot} - \bar{X})^2}^{\text{A}} + \overbrace{ac\sum_{j=1}^{b}(\bar{X}_{\cdot j\cdot} - \bar{X})^2}^{\text{B}} + \overbrace{c\sum_{k=1}^{c}(\bar{X}_{ij\cdot} - \bar{X}_{i\cdot\cdot} - \bar{X}_{\cdot j\cdot} + \bar{X})^2}^{\text{AB}} + \overbrace{\sum_{k=1}^{c}(x_{ijk} - \bar{X}_{ij\cdot})^2}^{\text{Error}}.$$

The hypotheses tests are as follow: $H_A : \alpha_1 = \alpha_2 = ... = \alpha_a = 0$, $H_B : \beta_1 = \beta_2 = ... = \beta_b = 0$, $H_{AB} : \gamma_{ij} = 0, \forall (i, j)$.

ANOVA Table

Source	SS	df	MS	F
Factor A	SS(A)	$a - 1$	$\frac{SS(A)}{a-1}$	$\frac{MS(A)}{MS(E)}$
Factor B	SS(B)	$b - 1$	$\frac{SS(B)}{b-1}$	$\frac{MS(B)}{MS(E)}$
Interaction AB	SS(AB)	$(a - 1)(b - 1)$	$\frac{SS(AB)}{(a-1)(b-1)}$	$\frac{MS(AB)}{MS(E)}$
Error	SS(E)	$ab(c - 1)$	$\frac{SS(E)}{ab(c-1)}$	
Total	SS(TOT)	$abc - 1$		

$F_1 \sim F(a - 1, ab(c - 1))$, $F_2 \sim F(b - 1, ab(c - 1))$, $F_3 \sim F((a - 1)(b - 1), ab(c - 1))$.

7.4.14 Linear Regression

Two random variablesX, Y. These are dependent random variables.

Example: X is SAT scores and Y is college GPA. $y = a + bx + \epsilon$

Example: X is the number of years of education. Y is the income of workers

Example: X is the height of a child at $2-1/2$ years old. Y is the height of an adult child.

$$y = bx + \epsilon.$$

Example: X is the expenditure on advertising. Y is the increase in sales. $y = a + bx + \epsilon$. $E(Y|x) = \mu(x), Y|x \sim N[\mu(x), \sigma^2]$. $\mu(x)$ is a linear function of x. $\mu(x) = \alpha+\beta(x-\bar{x})$, $y = \alpha+\beta(x-\bar{x})+\epsilon, \epsilon \sim N[0, \hat{\sigma}^2]$. $(y_1, x_1), (y_2, x_2), ...(y_n, x_n)$ is a random sample. Then, $y_i = \alpha+\beta(x_i-\bar{x})+\epsilon_i, i = 1, 2, ..., n$. Need to estimate α and β. The joint pdf of $y_1, y_2, ..., y_n$ for given $x_1, x_2, ..., x_n$. $\epsilon_1, \epsilon_2, ..., \epsilon_n \sim N(0, \sigma^2)$.

$$\left(\frac{1}{\sqrt{2\pi}\sigma}\right)^n e^{-\sum \frac{\epsilon_i^2}{2\sigma^2}} = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^n e^{\frac{-n}{2\sigma^2}\sum [Y_i-\alpha-\beta(x_i-\bar{x})]^2} = L(\alpha, \beta, \sigma^2|y_1, y_2, ..., y_n).$$

Maximizing L with respect to (α, β) is the same as minimizing

$$H(\alpha, \beta) = \sum_{i=1}^{n}[Y_i - \alpha - \beta(x_i - \bar{x})]^2.$$

$$\frac{\partial H}{\partial \alpha} = \sum_{i=1}^{n} -2[Y_i - \alpha - \beta(x_i - \bar{x})] = 0.$$

Since, $\sum_{i=1}^{n}(x_i - \bar{x}) = 0$, we have $\sum_{i=1}^{n} Y_i = \sum_{i=1}^{n} \alpha = \alpha n$. Thus, $\hat{\alpha} = \bar{Y}$.

$$\frac{\partial H}{\partial \beta} = \sum_{i=1}^{n} -2[x_i - \bar{x}][Y_i - \alpha - \beta(x_i - \bar{x})] = 0$$

$$\sum_{i=1}^{n}(x_i - \bar{x})Y_i - \alpha(x_i - \bar{x}) - \beta\sum_{i=1}^{n}(x_i - \bar{x})^2 = 0 \Rightarrow \hat{\beta} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}.$$

$Y = \bar{Y} + \hat{\beta}(x - \bar{x})$. The fitted line is $\hat{Y} = \bar{Y} + \hat{\beta}(x - \bar{x})$. For $x = x_i$, $\hat{Y}_i = \bar{Y} + \hat{\beta}(x_i - \bar{x})$.

$$\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2 = \sum_{i=1}^{n}[Y_i - \bar{Y} - \hat{\beta}(x_i - \bar{x})]^2.$$

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}{n}$$

which is the MLE of the variance.

Example: Problem 8.4-1 on page 492 of the text book. X is the score in preliminary test. Y is the score in the final test. $n = 10$.

$$\bar{X} = 68.3, \bar{Y} = 81.3, \sum_{i=1}^{n}(x_i - \bar{x})^2 = 756.1, \sum_{i=1}^{n} Y_i(x_i - \bar{x}) = 561.1, \hat{\beta} = \frac{561.1}{756.1} = 0.74.$$

The least square fitted line is $\hat{Y} = 81.3 + 0.74(x - 68.3) \Rightarrow \hat{Y} = 30.75 + 0.74x$. $\hat{Y}$ for $x = 75$ is 86.3.

7.4.15 Homework

7.3-2 Assume that the weight of cereal in a "10-ounce box" is $N(\mu, \sigma^2)$. To test $H_0 : \mu = 10.1$ against $H_1 : \mu > 10.1$, we take a random sample of size $n = 16$ and observe that $\bar{x} = 10.4$ and $s = 0.4$.

(a) Do we accept or reject H_0 at the 5% significance level? Reject H_0 if the following equation holds true:

$$\bar{x} \geq \mu_0 + \frac{t_\alpha(15)s}{\sqrt{16}}.$$

Substituting in the actual data yields, $10.4 \geq 10.1 + \frac{1.753(0.40)}{4}$, Since $10.4 \geq 10.2753$, the null hypothesis is rejected.

(b) What is the approximate p-value of this test? The test statistic is

$$t = \frac{(\bar{x} - 10.1)\sqrt{16}}{s} = 3.$$

According to Table IV, $p < 0.005$. The computer value of p is 0.0045.

7.3-12 In May the fill weights of 6-pound boxes of laundry soap had a mean of 6.13 pounds with a standard deviation of 0.095. The goal was to decrease the standard deviation. The company decided to adjust the filling machines and then test $H_0 : \sigma = 0.095$ against $H_1 : \sigma < 0.095$. In June a random sample of size $n = 20$ yielded $\bar{x} = 6.10$ and $s = 0.065$.

(a) At an $\alpha = 0.05$ significance level, was the company successful? If the company was successful, then the following equation would hold true:

$$P\left(s^2 \leq \frac{\sigma_0^2 \chi^2_{1-\alpha}(n-1)}{n-1}\right) = 1 - \alpha.$$

Substituting in the actual data yields, $0.065^2 \leq \frac{(0.095)^2(10.12)}{19}$. Since $0.004225 \leq 0.004807$, the null hypothesis is rejected. The company was successful in reducing the standard deviation.

(b) What is the approximate p-value of this test? The test statistic is given by the following equation:

$$\chi^2 = \frac{(n-1)s^2}{0.095^2} = 8.895.$$

Looking at Table III, $0.010 < p < 0.025$. A computer program gives $p = 0.025$.

7.3-13 The mean birth weight in the United States is $\mu = 3315$ grams with a standard deviation of $\sigma = 575$. Let X equal the birth weight in Rwanda. Assume that the distribution of X is $N(\mu, \sigma^2)$. We shall test the hypothesis $H_0 : \sigma = 575$ against the alternative hypothesis $H_1 : \sigma < 575$ at an $\alpha = 0.10$ significance level.

(a) What is your decision if a random sample of size $n = 81$ yielded $\bar{x} = 2819$ and $s = 496$? If the following inequality holds true, then the null hypothesis is rejected:

$$s^2 \leq \frac{\sigma_0^2 \chi^2_{1-\alpha}(n-1)}{n-1}.$$

Substituting in actual data yields, $496^2 \leq \frac{575^2(64.28)}{80}$. Since $246016 \leq 265657.1875$, the null hypothesis is rejected. An alternative way of looking at the problem is to solve for the χ^2 test statistic. Since $59.528 \leq 64.28$, the null hypothesis is rejected.

(b) What is the approximate p-value of this test? The test statistic is given as

$$\chi = \frac{(n-1)s^2}{\sigma_0^2} = \frac{80(496^2)}{575^2} = 59.528.$$

From the tables, $0.025 < p < 0.05$. The computer gives the value $p = 0.042$.

7.3-17 Each of 51 golfers hit three golf balls of brand X and three golf balls of brand Y in a random order. Let X_i and Y_i equal the averages of the distances traveled by the brand X and brand Y golf balls hit by the i-th golfer, $i = 1, 2, ..., 51$. Let $W_i = X_i - Y_i, i = 1, ..., 51$. Test $H_0 : \mu_W = 0$ against $H_1 : \mu_W > 0$, where μ_W is the mean of the differences. If $\bar{w} = 2.07$ and $s_W^2 = 84.63$, would H_0 be accepted or rejected at an $\alpha = 0.05$ level of significance? If the following inequality holds true, then the null hypothesis is rejected:

$$\bar{w} \geq \mu_0 + \frac{t_\alpha(n-1)s}{\sqrt{n}}.$$

Substituting in values yields, $2.07 \geq 0 + \frac{1.645\sqrt{84.63}}{\sqrt{51}}$. Since $2.119 > 2.07$, the null hypothesis is accepted. An alternative way of answering the question is to solve for the test statistic t.

$$t = \frac{(\bar{w} - \mu_0)\sqrt{n}}{s} = 1.607 < 1.645.$$

Since the inequality holds true, accept the null hypothesis.

7.3-18 To test whether a golf ball of brand A can be hit a greater distance off the tee than a golf ball of brand B, each of 17 golfers hit a ball of each brand, eight hitting ball A before ball B and nine hitting ball B before ball A. Assume that the differences of the paired A distance and B distance are approximately normally distributed and test the null hypothesis $H_0 : \mu_D = 0$ against the alternative hypothesis $H_1 : \mu_D > 0$ using a t-test with the 17 differences. Let $\alpha = 0.05$.

Golfer	Ball A	Ball B
1	265	252
2	272	276
3	246	243
4	260	246
5	274	275
6	263	246
7	255	244
8	258	245
9	276	259
10	274	260
11	274	267
12	269	267
13	244	251
14	212	222
15	235	235
16	254	255
17	224	231

Using the data in the above table, the following values can be calculated:

$$\bar{x} = \frac{81}{17} = 4.765, \ s^2 = \frac{1321.0588525}{16} = 82.566.$$

If the following inequality holds true then the null hypothesis is rejected:

$$\bar{x} \geq \mu_0 + \frac{t_\alpha(n-1)s}{\sqrt{n}}.$$

Substituting in actual values yields, $4.765 \geq 0 + \frac{1.746\sqrt{82.566}}{\sqrt{17}}$. Since $4.765 \geq 3.8479$, the null hypothesis is rejected. Alternatively, solve for the test statistic t. Since,

$$t = \frac{(4.765 - 0)\sqrt{n}}{\sqrt{82.566}} = 2.162 \geq 1.746,$$

the null hypothesis is rejected.

7.4-3 Among the data collected for the World Health Organization air quality monitoring project is a measure of suspended particles in $\mu g/m^3$. Let X and Y equal the concentration of suspended particles in $\mu g/m^3$ in the i-th center(commercial district), for Melbourne and Houston, respectively. Using $n = 13$ observations of X and $m = 16$ observations of Y, we shall test $H_0 : \mu_X = \mu_Y$ against $H_1 : \mu_X < \mu_Y$.

(a) Define the test statistic and critical region, assuming that the variances are equal. Let $\alpha = 0.05$. The test statistic is given by the following equation:

$$t = \frac{\bar{X} - \bar{Y}}{s_p\sqrt{\frac{1}{n} + \frac{1}{m}}} \leq -t_{0.05}(27),$$

where

$$s_p = \sqrt{\frac{(n-1)s_X^2 + (m-1)s_Y^2}{n+m-2}}.$$

(b) If $\bar{x} = 72.9$, $s_x = 25.6$, $\bar{y} = 81.7$, and $s_y = 28.3$, calculate the value of the test statistic and state your conclusion.

$$t = \frac{72.9 - 81.7}{27.1332(0.3734)} = -0.868576.$$

Since $-0.868576 > -1.703$, the null hypothesis is accepted.

(c) Give limits for the p-value of this test. According to the tables, $0.10 < p < 0.25$. The computer gives p as 0.1964.

(d) Test whether the assumption of equal variances is valid. Let $\alpha = 0.05$. The hypothesis being tested is as follow: $H_0 : \sigma_X = \sigma_Y$. versus $H_1 : \sigma_X \neq \sigma_Y$. If either of the following inequalities holds true, the null hypothesis is rejected:

$$\frac{s_X^2}{s_Y^2} \geq F_{\alpha/2}(n-1, m-1) = 2.96, \ \frac{s_Y^2}{s_X^2} \geq F_{\alpha/2}(m-1, n-1) = 3.18.$$

Since $0.8183 < 2.96$ and $1.22 < 3.18$, the null hypothesis is not rejected.

7.4.16 Correlation Coefficient

$$Y|x \sim N(\mu_x, \sigma^2), \ Y_i = \alpha + \beta(x_i - \bar{x}) + \epsilon_i, i = 1, 2, ..., n.$$

$$E(Y_i) = \alpha + \beta(x_i - \bar{x}), \ Var(Y_i) = \sigma^2, \forall i.$$

The least squares estimators are

$$\hat{\alpha} = \bar{Y}, \ \hat{\beta} = \frac{\sum_{i=1}^{n} Y_i(x_i - \bar{x})}{d^2},$$

where d^2 is $d^2 = \sum_{i=1}^{n}(x_i - \bar{x})^2$. The fitted line is $\hat{Y} = \bar{Y} + \hat{\beta}(x - \bar{x})$. $\hat{Y}$ is an estimate of Y for a given x. The correlation coefficient ρ is given by: $\rho = \frac{Cov(X,Y)}{\sqrt{Var(X)Var(Y)}}$. The sample correlation coefficient is $r = \frac{S_{xy}}{S_x S_y}$,

$$S_{xy} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}),\ S_x^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2.$$

$$S_{xy} = \frac{1}{n-1}\sum_{i=1}^{n} y_i(x_i - \bar{x}) - \sum_{i=1}^{n}\bar{y}(x_i - \bar{x}) = \frac{1}{n-1}\sum_{i=1}^{n} y_i(x_i - \bar{x})$$

$$\hat{\beta} = \frac{S_{xy}}{S_x^2} = \frac{S_{xy}}{S_x S_y}\left(\frac{S_x}{S_y}\right) \Rightarrow \hat{\beta} = r\frac{S_y}{S_x}, -1 \leq r \leq 1.$$

The correlation coefficient tells how good of a linear relationship exists.

$$E(\hat{\alpha}) = E(\bar{Y}) = E\left[\frac{1}{n}\sum_{i=1}^{n} Y_i\right] = \frac{1}{n}\sum_{i=1}^{n} E(Y_i) = \frac{1}{n}\sum_{i=1}^{n}(\alpha + \beta(x_i - \bar{x})) = \frac{1}{n}\sum_{i=1}^{n}\alpha + \beta\sum_{i=1}^{n}(x_i - \bar{x}) =$$

$$\frac{n\alpha}{n} = \alpha.$$

Thus $\hat{\alpha}$ is an unbiased estimator for α.

$$Var(\hat{\alpha}) = Var\left(\frac{1}{n}\sum_{i=1}^{n} Y_i\right) = \frac{1}{n^2}\sum_{i=1}^{n} Var(Y_i) = \frac{1}{n^2}\sum_{i=1}^{n}\sigma^2 = \frac{\sigma^2}{n}.$$

Thus $\hat{\alpha} \sim N(\alpha, \sigma^2/n)$.

$$E(\hat{\beta}) = E\left(\sum_{i=1}^{n} a_i Y_i\right), a_i = \frac{x_i - \bar{x}}{d^2},$$

$$E(\hat{\beta}) = \sum_{i=1}^{n} a_i E(Y_i) = \sum_{i=1}^{n} a_i(\alpha + \beta(x_i - \bar{x})) = \alpha\sum_{i=1}^{n} a_i + \beta\sum_{i=1}^{n}(x_i - \bar{x})a_i.$$

Note that

$$\sum_{i=1}^{n}(x_i - \bar{x})a_i = \frac{1}{d^2}\sum_{i=1}^{n}(x_i - \bar{x})(x_i - \bar{x}) = \frac{1}{d^2}\sum_{i=1}^{n}(x_i - \bar{x})^2 = \frac{d^2}{d^2} = 1.$$

So, $E(\hat{\beta}) = \beta$ is a unbiased estimator.

$$Var(\hat{\beta}) = Var\left(\sum_{i=1}^{n} a_i Y_i\right) = \sum_{i=1}^{n} a_i^2 Var(Y_i).$$

If $x_1, x_2, ..., x_n$ are independent and $a_1, a_2, ..., a_n$ are constants then,

$$\sigma^2\sum_{i=1}^{n} a_i^2 = \frac{\sigma^2}{d^4}\sum_{i=1}^{n}(x_i - \bar{x})^2 = \frac{\sigma^2 d^2}{d^4} = \frac{\sigma^2}{d^2}.$$

$$\hat{\beta} \sim N\left(\beta, \frac{\sigma^2}{d^2}\right).$$

7.4.17 Mid-term Exam

Do any 6 problems.

1. Let $X_1, X_2, ..., X_n$ be a random sample from a distribution with mean μ and variance σ^2. Prove that $S^2 = \frac{1}{n-1}\sum(X_i - \bar{X})^2$ is an unbiased estimator of σ^2.

2. Consider a random sample of size 13 from $N(\mu, 36)$. For testing $H_0 : \mu = 50$ against $H_1 : \mu > 50$, consider the test which rejects H_0 if $\bar{x} > 53$. Derive the power of this test for $H_1 : \mu = 55$. Answer: 0.8849.

3. Let p be the proportion of Americans who favor the death penalty. In a random sample of 1230 people, 750 favor the death penalty, 400 are against and 80 are indifferent. Find an approximate 95% confidence interval of p. Answer: [0.583,0.637].

4. Let X be Binomial(100,p). To test $H_0 : p = 0.08$ against $H_1 : p < 0.08$, we reject H_0 if $X \leq 6$.

   (a) Determine significance level α of this test. Answer: 0.2912.

   (b) Find Type II error for $H_1 : p = 0.06$. Answer: 0.417.

5. Standard deviation of weight of third grade children is 5 lbs. What should be the sample size n so that the sample mean is within one pound of μ with probability 0.95. You can assume that n is large. Answer: 96.

6. The pulse rate of a random sample of 15 workers from a mining town gives $\bar{x} = 82$ and $s^2 = 60$. Test if mean pulse rate of the mining workers is 75. Use $\alpha = 0.01$ and state H_1 and other assumptions. Answer: $t = 3.5, t_{0.005}(14) = 2.997$.

7. In a sampling poll for presidential election, what should be the sample size so that the maximum error in your estimate of p, the proportion of voters for a given candidate, is no more than 3% with probability 0.95. Answer: $n = 1067$.

8. Let the life of light bulbs be distributed as $N(\mu, \sigma^2)$. Based on a sample size 10 with $\bar{x} = 890, s^2 = 9200,$, test $H_0 : \sigma^2 = 9000$ against $H_1 : \sigma^2 > 9000$ with $\alpha = 0.025$. Answer: $\chi^2 = 9.2, \chi^2_{0.025}(9) = 19.0$.

7.5 Linear Model Test Statistics

$$Y_i = \alpha + \beta(x_i - \bar{x}) + \epsilon_i, i = 1, 2, ..., n,\ \hat{\alpha} = \bar{Y}, \hat{\beta} = \sum_{i=1}^{n} a_i Y_i,\ a_i = \frac{1}{d^2}\sum_{i=1}^{n}(x_i - \bar{x}).$$

$$d^2 = \sum_{i=1}^{n}(x_i - \bar{x})^2,\ \hat{Y}_i = \hat{\alpha} + \hat{\beta}(x_i - \bar{x}).$$

$$\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2,\ \tilde{\sigma}^2 = \frac{1}{n-2}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2,\ \hat{\beta} \sim N(\beta, \sigma^2/d^2).$$

$$Var(\hat{\beta}) = \frac{\sigma^2}{\sum_{i=1}^{n}(_i - \bar{x})^2},\ \frac{\sum_{i=1}^{n}\epsilon_i^2}{\sigma^2} = \frac{1}{\sigma^2}\sum_{i=1}^{n}(Y_i - \alpha - \beta(x_i - \bar{x}))^2,\ \epsilon_i \sim N(0, \sigma^2),\ \frac{\epsilon_i^2}{\sigma^2} \sim \chi_i^2.$$

Suppose σ^2 is unknown. Use $\tilde{\sigma}$ since it does not depend on σ^2.

$$\frac{1}{\sigma^2}\sum_{i=1}^{n}(Y_i - \alpha - \beta(x_i - \bar{x}))^2 = \frac{1}{\sigma^2}\sum_{i=1}^{n}[Y_i - \hat{Y}_i]^2 \sim \chi^2(n-2).$$

$H_0 : \beta = 0$. In general, $H_0 : \beta = \beta_0$. $\hat{\beta} \sim N(\beta_0, \sigma^2/d^2)$. $\frac{(\hat{\beta} - \beta_0)d}{\sigma} \sim N(0, 1)$. The test statistic is $\frac{(\hat{\beta} - \beta_0)d}{\tilde{\sigma}} = T \sim t(n-2)$. Reject H_0 if $T > t_\alpha(n-2)$ for $H_1 : \beta > \beta_0$.

The confidence interval of β is derived as follow:

$$\frac{(\hat{\beta}-\beta)d}{\tilde{\sigma}} \sim t(n-2),\ \hat{\beta} \pm t_{\alpha/2}(n-2)\frac{\tilde{\sigma}}{d}.$$

The length is $2t_{\alpha/2}(n-2)\frac{\tilde{\sigma}}{d}$.

Example: Problem 8.5-1 on page 499. $n=10, \hat{\beta}=0.742, \tilde{\sigma}^2=27.214, d^2=756.1$. $H_0:\beta=0$. $H_1:\beta\neq 0$. $t=\frac{(0.742-0)\sqrt{756.1}}{\sqrt{27.214}}=3.911$. At $\alpha=0.01, t_{0.005}(8)=3.3555$, reject H_0.

Putting the ANOVA variables into linear regression terms yields:

$$SS(TOT)=\sum_{i=1}^n (Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x})+\hat{\alpha}+\hat{\beta}(x_i-\bar{x})-\bar{Y})^2=\sum_{i=1}^n (Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x}))^2+\hat{\beta}^2\sum_{i=1}^n (x_i-\bar{x})^2.$$

$$\hat{\beta}\sum_{i=1}^n (x_i-\bar{x})(Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x}))=\hat{\beta}\left[\sum_{i=1}^n (x_i-\bar{x})Y_i-\hat{\beta}\sum_{i=1}^n (x_i-\bar{x})^2\right].$$

From the definition of $\hat{\beta}$, we have

$$\sum_{i=1}^n (x_i-\bar{x})Y_i-\hat{\beta}\sum_{i=1}^n (x_i-\bar{x})^2=0,\ \sum_{i=1}^n (Y_i-\bar{Y})^2=\overbrace{\sum_{i=1}^n (Y_i-\hat{Y}_i)^2}^{\text{error}}+\hat{\beta}^2\sum_{i=1}^n (x_i-\bar{x})^2.$$

$SS(TOT)=SS(E)+SS(R)$, where $SS(R)$ is the sum of squares due to regression. The variance in Y's is explained by linear regression.

$$\hat{\beta}^2\sum_{i=1}^n (x_i-\bar{x})^2=\hat{\beta}^2\sum_{i=1}^n (x_i-\bar{x})^2.$$

$$\left[\frac{\sum_{i=1}^n Y_i(x_i-\bar{x})}{\sum_{i=1}^n (x_i-\bar{x})^2}\right]^2\sum_{i=1}^n (x_i-\bar{x})^2=\frac{\left[\sum_{i=1}^n Y_i(x_i-\bar{x})\right]^2}{\sum_{i=1}^n (x_i-\bar{x})^2}=r^2\sum_{i=1}^n (Y_i-\bar{Y})^2 \Rightarrow \frac{SS(R)}{\sum_{i=1}^n (Y_i-\bar{Y})^2}=r^2.$$

That is the square of the sample correlation coefficient. $100r^2$ is the percentage of variation in Y explained by linear regression. The correlation coefficient is an indicator of linear dependence between x and y. $\sum_{i=1}^n (Y_i-\bar{Y})^2=\sum_{i=1}^n Y_i^2-n\bar{Y}^2$. $SS(E)=SS(TOT)-SS(R)$. $H_0:\beta=0$. $H_1:\beta\neq 0$.

Regression Table

Source	SS	df	MS	F
Regression	$\hat{\beta}^2\sum_{i=1}^n (x_i-\bar{x})^2$	1	SS(R)/1	MS(R)/MS(E)
Error	$\sum_{i=1}^n (Y_i-\hat{Y}_i)^2$	$n-2$	SS(E)/(n-2)	
Total	$\sum_{i=1}^n (Y_i-\bar{Y})^2$	$n-1$		

$MS(E)=\tilde{\sigma}^2$. $F\sim F_\alpha(1,n-2)$.

Example: Problem 8.5-2 on page 501 of the text book.

Source	SS	df	MS	F
Regression	416.39	1	416.39	15.3006
Error	217.71	8	27.214	
Total	634.10	9		

$F_{0.01} = 11.26$. Since $15.3006 > 11.26$, reject H_0. The percentage explained by regression is $\frac{416.39}{634.10}100 = 65.67\%$.

7.6 Homework and Answers

8.1-3 Four groups of three pigs were fed individually for different feeds for a specified length of time to test the hypothesis $H_0 : \mu_1 = \mu_2 = \mu_3 = \mu_4$, where μ_i is the mean weight gain for each of the feeds, $i = 1, 2, 3, 4$. Determine whether the null hypothesis is accepted or rejected at the %5 significance level if the observed weight gains are, respectively,

X_1 :	194.11	182.80	187.43	188.113
X_2 :	216.06	203.50	216.88	212.147
X_3 :	178.10	189.20	181.33	182.877
X_4 :	197.11	202.68	209.18	202.990
				196.53175

The ANOVA Table is as follow:

Source	d.f.	SS	MS	F
Treatment	3	1628.619	542.873	13.774
Error	8	315.2998	39.412	
Total	11	1943.919		

$F_{0.05}(3, 8) = 4.07$. Since $13.774 \geq 4.07$, reject H_0.

8.1-8 Let X_1, X_2, X_3, X_4 equal the cholesterol level of a woman under the age of 50, a man under 50, a woman 50 or older, and a man 50 or older, respectively. Assume that the distribution of X_i in $N(\mu_i, \sigma^2), i = 1, 2, 3, 4$. We shall test the null hypothesis $H_0 : \mu_1 = \mu_2 = \mu_3 = \mu_4$ using 7 observations of each X_i.

(a) Define a critical region for an $\alpha = 0.05$ significance level.

$$0.05 = P(F_{observed} \geq F_{0.05}(3, 24)),$$

or

$$0.05 = P\left(\frac{\frac{SS(T)}{3}}{\frac{SS(E)}{24}} \geq 3.01\right).$$

(b) Construct an ANOVA summary table and state your conclusion using the following data:

X_1 :	221	213	202	183	185	197	162	194.714
X_2 :	271	192	189	209	227	236	142	209.429
X_3 :	262	193	224	201	161	178	265	212.000
X_4 :	192	253	248	278	232	267	289	251.286
								216.8573

The ANOVA Table is as follow:

Source	d.f.	SS	MS	F
Treatment	3	12281.039	4093.680	3.4553
Error	24	28434.390	1184.766	
Total	27	40715.429		

$F_{0.05}(3, 24) = 3.01$. Since $3.4553 \geq 3.01$, the null hypothesis is rejected.

(c) Give bounds on the p-value for this test. $0.025 \leq p \leq 0.05$. The computer gives $p = 0.0323$.

8.2-4 Show that the cross-product terms formed from $\bar{X}_{i\cdot} - \bar{X}_{\cdot\cdot}$, $\bar{X}_{\cdot j} - \bar{X}_{\cdot\cdot}$, and $\bar{X}_{ij} - \bar{X}_{i\cdot} - \bar{X}_{\cdot j} + \bar{X}_{\cdot\cdot}$ sum to zero, $i = 1, 2, ..., a$ and $j = 1, 2, ..., b$.

Hint: For example, write

$$\sum_{i=1}^{a}\sum_{j=1}^{b}(\bar{X}_{\cdot j} - \bar{X}_{\cdot\cdot})(X_{ij} - \bar{X}_{i\cdot} + \bar{X}) = \sum_{j=1}^{b}(\bar{X}_{\cdot j} - \bar{X}_{\cdot\cdot})\sum_{i=1}^{a}(X_{ij} - \bar{X}_{\cdot j}) - (\bar{X}_{i\cdot} - \bar{X}_{\cdot\cdot}) =$$

$$\sum_{j=1}^{b}(\bar{x}_{\cdot j} - \bar{x}_{\cdot\cdot})[(a\bar{x}_{\cdot j} - a\bar{x}_{\cdot j}) - (a\bar{x}_{\cdot\cdot} - a\bar{x}_{\cdot\cdot})] = \sum_{j=1}^{b}(\bar{x}_{\cdot j} - \bar{x}_{\cdot\cdot})[0 - 0] = 0.$$

There are a total of 3 terms. Two terms have not been done.

8.2-5 A psychology student was interested in testing how food consumption by rats would be affected by a particular drug. She used two levels of one attribute, namely drug and placebo, and four levels of a second attribute, namely male (M), castrated (C), female (F), and ovariectomized (O). For each cell she observed five rats. The amount of food consumed in grams per 24 hours is listed in Table 8.2-8. Test the hypotheses using a 5% significance level for each.

Table 8.2-8

	M	C	F	O
Drug	22.56	16.54	18.58	18.20
	25.02	24.64	15.44	14.56
	23.66	24.62	16.12	15.54
	17.22	19.06	16.88	16.82
	22.58	20.12	17.58	14.56
Placebo	25.64	22.50	17.82	19.74
	28.84	24.48	15.76	17.48
	26.00	25.52	12.96	16.46
	26.02	24.76	15.00	16.44
	23.24	20.62	19.54	15.70

The means summary table is as follow:

	M	C	F	O	$\bar{X}_{i\cdot\cdot}$
Drug	22.208	20.996	16.920	15.936	19.015
Placebo	25.948	23.576	16.216	17.164	20.726
$X_{\cdot j\cdot}$	24.078	22.286	16.568	16.550	19.8705

The ANOVA Table is as follow:

Source	d.f.	SS	MS	F
A	1	29.27521	29.27521	5.533
B	3	454.69923	151.566	28.645
AB	3	27.34379	9.115	1.723
Error	32	169.31776	5.29118	
Total	39	680.63599		

(a) $H_{AB} : \gamma_{ij} = 0, i = 1, 2, j = 1, 2, 3, 4$. $F_{0.05}(3, 32) = 2.901$. Since $1.723 < 2.901$, the null hypothesis is not rejected.

(b) $H_A : \alpha_1 = \alpha_2 = 0$. Since $5.533 \geq 4.149$, the null hypothesis is rejected.

(c) $H_B : \beta_1 = \beta_2 = \beta_3 = \beta_4 = 0$. $F_{0.05}(1, 32) = 4.149$. Since $28.645 \geq 2.901$, the null hypothesis is rejected.

8.4-2 The final course grade in calculus was predicted on the basis of the student's high school grade point average in mathematics, Scholastic Aptitude Test(SAT) score in mathematics, and score on a mathematics entrance examination. The predicted grades X and the earned grades Y for 10 students are given(2.0 represents a C, 2.3 a C+, 2.7 a B-, etc.).

(a) Calculate the least squares regression line for these data. The sums are as follow:

$$\bar{x} = \frac{29}{10} = 2.9,\ \bar{y} = \frac{27.3}{10} = 2.73 = \hat{\alpha},\ \sum_{i=1}^{10}(x_i - \bar{x})^2 = 5.04,\ \sum_{i=1}^{10} y_i(x_i - \bar{x}) = 4.64.$$

From these sums, $\hat{\beta} = \frac{4.64}{5.04} = 0.921$. Thus, the fitted line is $\hat{y} = 2.73 + 0.921(x - 2.9)$.

(b) Plot the points and the least squares regression line on the same graph.

(c) Find the value of $\hat{\sigma}^2$.

$$\hat{\sigma}^2 = \frac{1}{10}\sum_{i=1}^{10}[y_i - \hat{\alpha} - \hat{\beta}(x_i - \bar{x})]^2 = \frac{1}{10}\sum_{i=1}^{10}[y_i - 2.73 - 0.921(x_i - \bar{x})]^2 = \frac{1.84925464}{10} = 0.185.$$

x	y	x	y
2.0	1.3	2.7	3.0
3.3	3.3	4.0	4.0
3.7	3.3	3.7	3.0
2.0	2.0	3.0	2.7
2.3	1.7	2.3	3.0

8.4-4 Show that

$$\sum_{i=1}^{n}[Y_i - \alpha - \beta(x_i - \bar{X})]^2 = n(\hat{\alpha} - \alpha)^2 + (\hat{\beta} - \beta)^2 \sum_{i=1} n(x_i - \bar{x})^2 + \sum_{i=1}^{n}[Y_i - \hat{\alpha} - \hat{\beta}(x_i - \bar{x})]^2.$$

Equation 8.4-5 on page 494 of the text book will be used.

$$\sum_{i=1}^{n}[(\hat{\alpha}-\alpha)+(\hat{\beta}-\beta)(x_i+\bar{x})+[Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x})]]^2 =$$

$$\sum_{i=1}^{n}(\hat{\alpha}-\alpha)^2+(\hat{\alpha}-\alpha)(\hat{\beta}-\beta)(x_i-\bar{x})+(\hat{\alpha}-\alpha)[Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x})]+$$

$$(\hat{\alpha}-\alpha)(\hat{\beta}-\beta)(x_i-\bar{x})+(\hat{\beta}-\beta)^2(x_i-\bar{x})^2+(\hat{\beta}-\beta)(x_i-\bar{x})[Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x})]+$$

$$(\hat{\alpha}-\alpha)[Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x})]+(\hat{\beta}-\beta)(x_i-\bar{x})[Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x})]+[Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x})]^2 =$$

$$n(\hat{\alpha}-\alpha)^2+n(\hat{\beta}-\beta)^2\sum_{i=1}^{n}(x_i-\bar{x})^2+\sum_{i=1}^{n}2(\hat{\alpha}-\alpha)(\hat{\beta}-\beta)(x_i-\bar{x})+$$

$$2(\hat{\alpha}-\alpha)[Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x})]+2(\hat{\beta}-\beta)(x_i-\bar{x})[Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x})]+[Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x})]^2 =$$

$$n(\hat{\alpha}-\alpha)^2+n(\hat{\beta}-\beta)^2\sum_{i=1}^{n}(x_i-\bar{x})^2+0+0+[Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x})]^2.$$

Let's see why some of the inner terms sum to zero. The following expression sums to zero because it is simply a constant multiplied by $(x_i-\bar{x})$. It is known that $(x_i-\bar{x})$ becomes $n\bar{x}-n\bar{x}=0$. $2(\hat{\alpha}-\alpha)(\hat{\beta}-\beta)(x_i-\bar{x})$. The following term sums to zero for two reasons: (1) the sum of $Y_i=n\bar{Y}$, and the sum of $\hat{\alpha}=n\bar{Y}$. Then, we have $n\bar{Y}-n\bar{Y}=0$, (2) for the same reason in the previous expression, a constant times $(x_i-\bar{x})=0$. $2(\hat{\alpha}-\alpha)[Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x})]$ And finally the term, $2(\hat{\beta}-\beta)(x_i-\bar{x})[Y_i-\hat{\alpha}-\hat{\beta}(x_i-\bar{x})]$. We know that $Y_i(x_i-\bar{x})$ is the same as $\hat{\beta}(x_i-\bar{x})^2$ by definition of $\hat{\beta}$. Thus, $\hat{\beta}(x_i-\bar{x})^2-\hat{\beta}(x_i-\bar{x})^2=0$. That only leaves $(x_i-\bar{x})$ being multiplied by a constant which is going to sum to zero from previous explanations.

8.5-2 For the data given in Exercise 8.4-2,

(a) Test $H_0:\beta=0$ against $H_1:\beta>0$ at the $\alpha=0.025$ significance level using a t-test. The test statistic is

$$T_1=\frac{\hat{\beta}-\beta_0}{\sqrt{\frac{n\hat{\sigma^2}}{(n-2)\sum(x_i-\bar{x})^2}}}=\frac{0.921-0}{\sqrt{\frac{10(0.185)}{8(5.04)}}}=4.2997.$$

$t_\alpha(n-2)=t_{0.025}(8)=2.306$. Since $4.2997\geq 2.306$, the null hypothesis is rejected.

(b) Test $H_0:\beta=0$ against $H_1:\beta\neq 0$ at the $\alpha=0.05$ significance level by setting up the ANOVA table and using an F statistic.

Source	d.f.	SS	MS	F
Regression	1	4.2751	4.2751	18.528
Error	8	1.8459	0.2307375	
Total	9	6.121		

Since $18.528\geq F_{0.05}(1,8)=5.32$, the null hypothesis is rejected.

(c) Find a 95% confidence interval for $\mu_{Y|x}$ when $x = 2, 3, 4$.

- $*$ For $x = 2$:

$$2.73 + 0.921(2 - 2.9) \pm \left[\sqrt{\frac{10(0.185)}{8}}\sqrt{\frac{1}{10} + \frac{(2-2.9)^2}{5.04}}\right](2.306) = 1.9011 \pm 0.5662.$$

- $*$ For $x = 3 : 2.8221 \pm 0.3541$.
- $*$ For $x = 4 : 3.7431 \pm 0.6467$.

(d) Find a 95% prediction interval for Y when $x = 2, 3, 4$.

- $*$ For $x = 2 : 1.9011 \pm 1.2451$.
- $*$ For $x = 3 : 2.8221 \pm 1.1641$.
- $*$ For $x = 4 : 3.7431 \pm 1.2837$.

8.5-8 A computer center recorded the number of programs it maintained during each of 10 consecutive years.

(a) Calculate the least squares regression line for these data. The sums are as follow:

$$\bar{x} = \frac{55}{10} = 5.5, \ \bar{y} = \frac{9811}{10} = 981.1 = \hat{\alpha},$$

$$\sum_{i=1}^{10}(x_i - \bar{x})^2 = 82.5, \ \sum_{i=1}^{10} y_i(x_i - \bar{x}) = 11589.5.$$

$\hat{\beta} = \frac{11589.5}{82.5} = 140.479$. The least squares line is $\hat{y} = 981.1 + 140.479(x - 5.5)$.

(b) Plot the points and the line on the same graph.

(c) Find a 95% prediction interval for the number of programs in year 11 under the usual assumptions. First solve for $\hat{\sigma}^2$.

$$\hat{\sigma}^2 = \sum_{i=1}^{10}[y_i - 981.1 - 140.479(x_i - 5.5)]^2 = 26377.8.$$

The prediction interval is,

$$981.1 + 140.479(11 - 5.5) \pm \left[\sqrt{\frac{10(26377.8)}{8}}\sqrt{1.1 + \frac{(11-5.5)^2}{82.5}}\right](2.306) = 1753.735 \pm 507.11.$$

Year	No. Programs
1	430
2	480
3	565
4	790
5	885
6	960
7	1200
8	1380
9	1530
10	1591

7.7 Confidence Interval of Y and E(Y)

$Y = \alpha + \beta(x-\bar{x}) + \epsilon,\ E(Y) = \alpha + \beta(x-\bar{x}) = \mu(x)$. $\hat{Y} = \hat{\alpha} + \hat{\beta}(x-\bar{x}) = \bar{Y} + \hat{\beta}(x-\bar{x})$, which is an estimator for $\mu(x)$ as well as Y.

$$E(\hat{Y}) = \mu(x),\ \hat{Y} = \sum_{i=1}^{n}\left[\frac{1}{n} + (x-\bar{x})a_i\right]Y_i,$$

$$Var(\hat{Y}) = \sum_{i=1}^{n}\left[\frac{1}{n} + (x-\bar{x})a_i\right]^2 Var(Y_i) = \sigma^2\sum_{i=1}^{n}\left[\frac{1}{n^2} + (x-\bar{x})^2a_i^2 + \frac{2}{n}(x-\bar{x})a_i\right] = \sigma^2\left[\frac{1}{n} + \frac{(x-\bar{x})^2}{d^2}\right].$$

$$\hat{Y} \sim N\left(\mu(x), \sigma^2\left[\frac{1}{n} + \frac{(x-\bar{x})^2}{d^2}\right]\right),\ \tilde{\sigma}^2 = \frac{1}{n-2}\sum_{i=1}^{n}(Y_i - \hat{Y})^2.$$

The test statistic is

$$T = \frac{\hat{Y} - \mu(x)}{\tilde{\sigma}\sqrt{\frac{1}{n} + \frac{(x-\bar{x})^2}{d^2}}} \sim t(n-2).$$

A $(1-\alpha)100\%$ confidence interval of $\mu(x)$ is

$$\hat{Y} \pm \tilde{\sigma}\sqrt{\frac{1}{n} + \frac{(x-\bar{x})^2}{d^2}}$$

The confidence interval for Y itself is

$$E(Y - \hat{Y}) = E(Y) - E(\hat{Y}) = 0.$$

$$Var(Y - \hat{Y}) = Var(Y) + Var(\hat{Y}) = \sigma^2\left[1 + \frac{1}{n} + \frac{(x-\bar{x})^2}{d^2}\right].$$

Therefore,

$$Y - \hat{Y} \sim N\left(0, \sigma^2\left[1 + \frac{1}{n} + \frac{(x-\bar{x})^2}{d^2}\right]\right).$$

The test statistic is

$$T = \frac{Y - \hat{Y}}{\sqrt{1 + \frac{1}{n} + \frac{(x-\bar{x})^2}{d^2}}}.$$

The $(1-\alpha)100\%$ confidence interval of Y is

$$\hat{Y} \pm t_{\alpha/2}(n-2)\tilde{\sigma}\sqrt{1 + \frac{1}{n} + \frac{(x-\bar{x})^2}{d^2}}.$$

Example: Problem 8.5-3 on page 595 of the text book. $n = 10, \bar{x} = 68.3, \hat{\alpha} = 81.3, d^2 = 756.1, \hat{\beta} = 0.7421, \tilde{\sigma}^2 = \frac{n}{n-2}\hat{\sigma}^2 = 27.21$. For $x = 60$, estimate y and $\mu(x)$, and find the confidence interval. $\hat{y} = 81.3 + 0.7421(60 - 68.3) = 75.14$. The confidence interval is

$$c = \tilde{\sigma}\sqrt{\frac{1}{n} + \frac{(x-\bar{x})^2}{d^2}} = 27.2\sqrt{\frac{1}{10} + \frac{(60-68.3)^2}{756.1}} = 2.281.$$

$t_{0.025}(8) = 2.306$. $75.14 \pm 2.306(2.281) = [69.88, 80.40]$.

7.8 Multivariate Hypergeometric Distribution

Read Section 5.1 in the text book. There are k types of objects, n_i is the number of i-th types, $i = 1, 2, ..., k$. Choose r objects out of n_i different types. $n = \sum_{i=1}^{k} n_i$. Select r out of n. $\binom{\text{n}}{\text{r}}$ is the total number of ways to select r out of n. x_i is the number of objects of type i in the selection. The joint pdf of $x_1, x_2, ..., x_k$ is

$$f(x) = P(X_1 = x_1, X_2 = x_2, ..., X_k = x_k) = \frac{\binom{n_1}{x_1}\binom{n_2}{x_2}\binom{...}{...}\binom{n_k}{x_k}}{\binom{n}{r}}$$

$$\sum_{i=1}^{k} x_i = r, 0 \leq x_i \leq n_i.$$

Example: What is the probability of getting 2 spades, 3 diamonds, 4 hearts, and 4 clubs in a bridge hand.

$$\frac{\binom{13}{2}\binom{13}{3}\binom{13}{4}\binom{13}{4}}{\binom{52}{13}}$$

7.9 Multinomial Distribution

An experiment has k mutually exclusive and independent and exhaustive outcomes $A_1, A_2, ..., A_k$.

$$A_1 \cup A_2 \cup ... \cup A_k = S,\ P(A_i) = p_i, k = 1, ..., k,\ \sum_{i=1}^{k} p_i = 1.$$

Repeat the experiment n times. x_i is the number of times A_i happens out of n trials.

$$f(x) = P(X_1 = x_1, X_2 = x_2, ..., X_k = x_k) = \frac{n!}{x_1!x_2! \cdots x_k!} p_1^{x_1} p_2^{x_2} \cdots p_k^{x_k}$$

If there are only 2 outcomes, then use

$$\frac{n!}{k!(n-k)!},\ \sum_{i=1}^{k} x_i = n, 0 \leq x_i \leq n,\ 1 = (p_1 + p_2 + \cdots + p_k)^n = \sum_{i=1}^{k} \frac{n!}{x_1! \cdots x_k!} p_1^{x_1} p_2^{x_2} \cdots p_k^{x_k}.$$

Note that p_i is the same for all trials.

Example: Suppose there are n students from ODU. A_i happens if the student is in the i-th year, $i = 1, 2, 3, 4$. x_i is the number of students who belong to A_i in our selection. Suppose that,

p_1	p_2	p_3	p_4
30%	27%	23%	20%

For $n = 15$, $P(X_1 = 5, X_2 = 4, X_3 = 3, X_4 = 3) = \frac{15!}{5!4!3!3!}(0.30)^5(0.27)^4(0.23)^3(0.20)^3$. The marginal distribution of x_i, where $x_i \sim Binomial(n, p_i)$ is $E(x_i) = np_i; Var(x_i) = np_i(1 - p_i)$.
The multinomial distribution pdf can be written as:

$$f(x_1, x_2, ..., x_n) = \frac{n!}{\prod_{i=1}^{n} x_i!} \prod_{i=1}^{n} p_i^{x_i},\ \sum_{i=1}^{k} n_i = n.$$

The trinomial distribution is given by: $\frac{n!}{x_1!x_2!x_3!}p_1^{x_1}p_2^{x_2}p_3^{x_3}$, or using 2 random variables: $x_3 = n - x_1 - x_2 = n - x - y$, $p_3 = 1 - p_1 - p_2$. So we have, $\frac{n!}{x!y!(n-x-y)!}p_1^x p_2^y (1-p_1-p_2)^{n-x-y}$, $x = 0, 1, 2, ...n; y = 0, 1, 2, ...n; 0 \leq x + y \leq n$.

Example: In a poll, X is the voters for candidate A, Y is the voters for candidate B, and $n - X - Y$ are undecided voters.

Example: Select a committee of 10 students x_i is the number of students in the year $i, i = 1, 2, 3, 4$. For small n the distribution is Multivariate Hyper Geometric. For large n, the distribution is Multinomial.

For a Bivariate distribution, $\begin{pmatrix} \text{X} \\ \text{Y} \end{pmatrix}$, $\sigma_x^2 = Var(X)$, $\sigma_y^2 = Var(Y)$. $\mu_x = E(X)$, $\mu_y = E(Y)$. $f(x, y)$ is the joint pdf of X and Y. The *covariance* of (x, y) is

$$Cov(x, y) = E[(x - \mu_x)(y - \mu_y)] =$$

$$E[xy - x\mu_y - y\mu_x + \mu_x\mu_y] = E(xy) - \mu_x\mu_y - \mu_y\mu_x + \mu_x\mu_y = E(xy) - \mu_x\mu_y.$$

$E(xy) = \sum_Y \sum_X xyf(x, y)$. ρ_{xy} is the correlation coefficient of (x, y).

$$\rho_{xy} = \frac{Cov(x, y)}{\sqrt{Var(X)Var(Y)}} = \frac{\sigma_{xy}}{\sigma_x\sigma_y}.$$

If x and y are independent then, $E(XY) = E(X)E(Y) = \mu_x\mu_y$, $\sigma_{xy} = 0, \rho_{xy} = 0$. Independence of $x_1, x_2, ..., x_k$: By definition,

$$f(x_1, x_2, ..., x_k) = \prod_{i=1}^{k} f_i(x_i),$$

where $f_i(x_i)$ is the marginal pdf of x_i.

1. $-1 \leq \rho_{xy} \leq 1$.
2. $x^* = aX + b, y^* = cY + d$.

a, b, c, d are known constants. Assume that $a, c > 0$. Then, $\rho_{x^*y^*} = \rho_{xy}$. Note that the correlation coefficient is *scale independent and location independent.*

Proof:

$$\mu_{x^*} = a\mu_x + b,\ \mu_{y^*} = c\mu_y + d,\ \sigma_{x^*}^2 = a^2\sigma_x^2,\ \sigma_{y^*}^2 = c^2\sigma_y^2.$$

$$\sigma_{x^*y^*} = E[(x^* - \mu_{x^*})(y^* - \mu_{y^*})] = E[[(aX + b - (a\mu_x + b)][cY + d - (c\mu_y + d)]] =$$

$$acE[(x - \mu_x)(y - \mu_y)] = ac\sigma_{xy}.$$

$$\rho_{x^*y^*} = \frac{\sigma_{x^*y^*}}{\sigma_{x^*}\sigma_{y^*}} = \frac{ac\sigma_{xy}}{a\sigma_x c\sigma_y} = \rho_{xy}.$$

The best line thru (μ_x, μ_y) is $Y = \mu_x + b(x - \mu_x)$. Find b which minimizes $E(Y - \mu_y - b(x - \mu_x))^2 = K(b)$. $K(b) = E[(y - \mu_y)^2 + b^2(x - \mu_x)^2 - 2b(x - \mu_x)(y - \mu_y)] = \sigma_y^2 + b^2\sigma_x^2 - 2b\sigma_{xy}$.

$$\frac{\partial K}{\partial b} = 2b\sigma_x^2 - 2\sigma_{xy} = 0 \Rightarrow b^* = \frac{\sigma_{xy}}{\sigma_x^2} = \rho\frac{\sigma_y}{\sigma_x}.$$

The best line is $Y = \mu_y + \rho\frac{\sigma_y}{\sigma_x}(x - \mu_x)$.

$$K(b^*) = \sigma_y^2 + \rho^2\frac{\sigma_y^2}{\sigma_x^2}\sigma_x^2 - 2\frac{\rho\sigma_y\sigma_{xy}}{\sigma_x} = \sigma_y^2 + \rho^2\sigma_y^2 - 2\rho\frac{\sigma_y}{\sigma_x}\rho\sigma_x\sigma_y = \sigma_y^2(1 - \rho^2).$$

Remember that $K(b) \geq 0$. Then, $(1-\rho^2) \geq 0$, and $-1 \leq \rho \leq 1$. $\rho = \pm 1$ implies all the (x, y) points must lie on the line.

Example: x, y are dependent but $\rho = 0$.

x	y	0	1
0	0	$\frac{1}{3}$	$\frac{1}{3}$
1	$\frac{1}{3}$	0	$\frac{1}{3}$
2	0	$\frac{1}{3}$	$\frac{1}{3}$
	$\frac{1}{3}$	$\frac{2}{3}$	

,

x	y	$f(x, y)$
0	1	$\frac{1}{3}$
1	0	$\frac{1}{3}$
2	1	$\frac{1}{3}$

,

X	$f(x)$
0	$\frac{1}{3}$
1	$\frac{1}{3}$
2	$\frac{1}{3}$

,

Y	$f(y)$
0	$\frac{1}{3}$
1	$\frac{2}{3}$

$$E(XY) = \frac{2}{3} = 0\left(\frac{1}{2}\right) + 0\left(\frac{1}{3}\right) + 2\left(\frac{1}{3}\right), \ \sigma_{xy} = E(XY) - \mu_x\mu_y = \frac{2}{3} - 1\left(\frac{2}{3}\right) = 0.$$

$\mu_x = 1, \mu_y = \frac{2}{3}$. Thus, $\rho_{xy} = 0$. For x and y to be independent, $f(x, y) = f_1(x)f_2(y), \forall(x, y)$. Since $P(X = 0, Y = 0) \neq P(X = 0)P(Y = 0)$, x, y are not independent.

7.10 Conditional Distributions

Example: X is the height of adults. Y is the weight of adults. $f(x, y)$ is the joint pdf of x and y. The distribution of weights only for 5'10" adults is $x = 70$. $P(Y = y|x = 70) = h(Y|x = 70)$, $h(Y|x)$ is the conditional distribution of Y given x. $P(B|A) = \frac{P(B \cap A)}{P(A)}$. So, $h(Y|x) = \frac{f(x,y)}{f_1(x)}$.

Example: Suppose Y is adult height. X is the height at 2 years old. $E(Y|X = x) = 2x$, is given. $E(Y|X = x) = \sum_Y yh(Y|x)$. $\sum_Y h(Y|x) = 1$.

Example: $f(x, y) = \frac{x+y}{21}, x = 1, 2, 3; y = 1, 2.$

X/Y	1	2	Marginal
1	$\frac{2}{21}$	$\frac{3}{21}$	$\frac{5}{21}$
2	$\frac{3}{21}$	$\frac{4}{21}$	$\frac{7}{21}$
3	$\frac{4}{21}$	$\frac{5}{21}$	$\frac{9}{21}$
	$\frac{9}{21}$	$\frac{12}{21}$	

$$f_1(x) = \sum_{y=1}^{2} f(x, y) = \sum_{y=1}^{2} \frac{x+y}{21} = \frac{2x+3}{21}, x = 1, 2, 3.$$

$$h(Y|x) = \frac{f(x, y)}{f_1(x)} = \frac{\frac{x+y}{21}}{\frac{2x+3}{21}} = \frac{x+y}{2x+3}, y = 1, 2.$$

In general, do not read the tables for conditional probabilities. Use the derived equation. If x, y are independent, then $h(Y|x) = f_2(y)$.

7.11 Conditional Mean and Variance

$h(Y|x)$ is the conditional distribution of Y given x.

$$E(Y|x) = \sum_Y yh(Y|x),\ Var(Y|x) = \sum_Y y^2 h(Y|x) - [E(Y|x)]^2.$$

Example: Using the example in the last lecture,

$$f(x,y) = \frac{x+y}{21}, x = 1,2,3; y = 1,2,\ h(Y|x) = \frac{x+y}{2x+3}.$$

$$E(Y|x) = \sum_{y=1}^{2} y\left(\frac{x+y}{2x+3}\right) = \frac{x+1}{2x+3} + 2\left(\frac{x+2}{2x+3}\right) = \frac{3x+5}{2x+3}.$$

If $E(Y|x) = a + bX$, then

$$b = \frac{\rho\sigma_y}{\sigma_x},\ a = \mu_y - \frac{\rho\sigma_y}{\sigma_x}\mu_x,\ E(Y|x) = \mu_y + \frac{\rho\sigma_y}{\sigma_x}(x-\mu_x),$$

This is also the best line thru μ_x and μ_y.

Proof:

$$\sum_Y yh(Y|x) = a + bX.$$

$$f_1(x)\sum_Y \frac{yf(x,y)}{f_1(x)} = (a+bX)f_1(x).$$

Sum over x :

$$\sum_Y\sum_X yf(x,y) = a\sum_X f_1(x) + b\sum_X xf_1(x),\ \mu_y = a + b\mu_x.$$

$$\sum_Y\sum_X xyf(x,y) = a\sum xf_1(x) + b\sum x^2 f_1(x) = a\mu_x + b(\sigma_x^2 + \mu_x^2),$$

$$\sigma_{xy} = \rho\sigma_x\sigma_y,\ \mu_x\mu_y + \rho\sigma_x\sigma_y = a\mu_x + b(\sigma_x^2+\mu_x^2),\ \mu_y = a + b\mu_x,\ a = \mu_y - b\mu_x.$$

Example: Trinomial Distribution. X is the number of democrats. Y is the number of republicans. $Z = n - X - Y$ is the number of independents. $f(x,y) = \frac{n!}{x!y!(n-x-y)!}p_1^x p_2^y(1-p_1-p_2)^{(n-x-y)}$. $p_1+p_2+p_3 = 1$. The marginal is $Y \sim Binomial(n, p_2)$. The conditional distribution of $Y|x \sim Binomial(n^*, p^*)$. $n^* = n - x; p^* = \frac{p_2}{1-p_1}$. $Y|x \sim Binomial\left(n-x, \frac{p_2}{1-p_1}\right)$.

$$h(Y|x) = \frac{f(x,y)}{f_1(x)} =$$

$$\frac{n!}{x!y!(n-x-y)!}\frac{p_1^x p_2^y(1-p_1-p_2)^{(n-x-y)}}{\frac{N!}{x!(n-x)!}p_1^x(1-p_1)^{n-x}} = \frac{(n-x)!}{y!(n-x-y)!}\left(\frac{p_2}{1-p_1}\right)^y\left(1-\frac{p_2}{1-p_1}\right)^{n-x-y}$$

because $(1-p_1)^x = (1-p_1)^y(1-p_1)^{n-x-y}$. Then, $Y|x \sim Binomial\left(n-x, \frac{p_2}{1-p_2}\right)$. This is linear and so, $\mu_y + \frac{\rho\sigma_y}{\sigma_x}(x-\mu_x) = (n-x)\frac{p_2}{1-p_1}$. Therefore,

$$\rho = -\frac{p_2}{1-p_1}\frac{\sigma_x}{\sigma_y} = -\frac{p_2}{1-p_1}\sqrt{\frac{(np_1(1-p_1))}{np_2(1-p_2)}} = -\sqrt{\frac{p_1p_2}{(1-p_1)(1-p_2)}}.$$

7.12 Bivariate Normal Distribution

X and Y have a bivariate Normal distribution if,

$$f(x,y) = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-\rho^2}}e^{-\frac{1}{2}g(x,y)},$$

$$g(x,y) = \frac{1}{(1-\rho^2)}\left[\left(\frac{(x-\mu_y)}{\sigma_x}\right)^2 - 2\rho\left(\frac{x-\mu_x}{\sigma_x}\right)\left(\frac{y-\mu_y}{\sigma_y}\right) + \left(\frac{y-\mu_y}{\sigma_y}\right)^2\right], -\infty < x < \infty; -\infty < y < \infty.$$

ρ is the correlation coefficient of (x,y). The graph is bell shaped in 3-D. The marginal random variables are $X \sim N(\mu_x, \sigma_x^2)$, $Y \sim N(\mu_y, \sigma_y^2)$. If $\rho = 0$ the x and y are independent in the Normal case only. The conditional random variables are $Y|x \sim N(a+bX, \sigma_{Y|x}^2)$, $E(Y|x) = a+bX = \mu_y + \rho\frac{\sigma_y}{\sigma_x}(x-\mu_x)$. $Var(Y|x) = \sigma_y^2(1-\rho^2) < \sigma_y^2$. If $\rho = 1$ or -1, then (μ_x, μ_y) lies on the line $a + bX$.

Example: X is the high school GPA. Y is the college GPA at graduation. Given, $\mu_x = 2.9, \mu_y = 2.4, \sigma_x = 0.40, \sigma_y = 0.50, \rho = 0.80$. X and Y have a bivariate Normal distribution.

$$E(Y|x) = \mu_y + \rho\frac{\sigma_y}{\sigma_x}(x-\mu_x) = 2.4 + 0.80\left(\frac{0.50}{0.40}\right)(x-2.9) = x - 0.50.$$

Then, $E(Y|x = 3.0) = 2.5$.

7.13 Correlation Analysis

$\rho =$ correlation $(x,y) = \frac{\sigma_{xy}}{\sigma_x\sigma_y}$. The Bivariate random sample is,

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix}\begin{pmatrix} x_2 \\ y_2 \end{pmatrix}\begin{pmatrix} \dots \\ \dots \end{pmatrix}\begin{pmatrix} x_n \\ y_n \end{pmatrix}.$$

S_{xy} is the sample covariance.

$$S_{xy} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y}) = \frac{1}{n-1}\sum_{i=1}^{n}x_iy_i - \frac{n}{n-1}\bar{x}\bar{y}.$$

$$R = \frac{S_{xy}}{S_xS_y},\ \hat{\beta} = \frac{RS_y}{S_x}, -1 < R < 1.$$

If x and y have a bivariate Normal distribution, then $H_0 : \rho = 0$. The test statistic is

$$T = \frac{R\sqrt{n-2}}{\sqrt{1-R^2}} \sim t(n-2),$$

if H_0 is true. The distribution of R is given by

$$g(r) = \frac{\Gamma\left(\frac{n-1}{2}\right)}{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{n-2}{2}\right)}(1-r^2)^{\frac{n-4}{2}}.$$

For $H_1 : \rho \neq 0$, reject if $|T| > t_{\alpha/2}(n-2)$.

Example: Problem 9.4-1 on page 544 of the text book. $n = 18$. $H_0 : \rho = 0$. $H_1 : \rho \neq 0$. $r = 0.35, \alpha = 0.05, t_{0.025}(16) = 2.120$.

$$T = \frac{r}{\sqrt{1-r^2}}\sqrt{n-2} = \sqrt{16}\frac{0.35}{\sqrt{1-0.35^2}} = 1.495.$$

Thus, accept H_0 since $1.495 \leq 2.120$.

For large n only$(n > 30)$: $H_0 : \rho = \rho_0$. $H_1 : \rho \neq \rho_1$.

$$W = \frac{1}{2}\log\left(\frac{1+R}{1-R}\right) \sim N\left(\frac{1}{2}\log\frac{1+p_0}{1-p_0}, \frac{1}{n-3}\right), \quad z = \frac{W - \frac{1}{2}\log\left(\frac{1+p_0}{1-p_0}\right)}{\sqrt{\frac{1}{n-3}}} \sim N(0,1),$$

if H_0 is true. Reject H_0 if $|z| > z_{\alpha/2}$. For large n, $R \sim N(p_0, U(p_0))$. But, the variance is dependent on p_0. This is not the case for z.

7.14 Testing About the Distribution

Is the distribution of x Normal? Use the multinomial distribution. $(y_1, y_2, ..., y_k) \sim Multinomial(n, p_1, p_2, ..., p_k)$. $H_0 : p_i = p_i^*, i = 1, 2, ..., k$. For large n,

$$Q_{k-1} = \sum_{i=1}^{k} \frac{(Y_i - np_i^*)^2}{np_i^*} \to \chi^2(k-1).$$

y_i is the observed frequency of the i-th class, O_i. $np_i^* = E(Y_i) = E_i, Y_i \sim Binomial(n, p_i^*)$.

$$Q_{k-1} = \sum_{i=1}^{k} \frac{(O_i - E_i)^2}{E_i}.$$

That is called the *chi-squared goodness of fit test.* If p_i^* is not the correct probability, $Y_i \sim np_i$, and $Y_i - np_i \approx n(p_i - p_i^*)$.

Example: Throw a die 120 times. $H_0 : p_i = \frac{1}{6}, i = 1, 2, 3, 4, 5, 6$. $H_1 : p_i \neq \frac{1}{6}$, for at least one i.

outcome:	1	2	3	4	5	6
Y_i	26	13	21	29	20	11
p_i	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$
np_i	20	20	20	20	20	20

$$q_{k-1} = \sum_{i=1}^{6} \frac{(Y_i - np_i)^2}{np_i} = \frac{(26-20)^2}{20} + \frac{(13-20)^2}{20} + \cdots + \frac{(11-20)^2}{20} = 12.4$$

$\alpha = 0.05$, $\chi^2_{0.05}(5) = 11.07$. Since $12.4 > 11.07$, reject H_0. How to use the above test for other distributions? $H_0 : X \sim f(x|\theta)$. $x_1, x_2, ..., x_n$ is a random sample from a distribution with pdf $f(x|\theta)$. $p_i(\theta) = P(c_{i-1} < X < c_i) = F(c_i|\theta) - F(c_{i-1}|\theta)$, where $F(x|\theta) = P(X \leq x)$. y_i is the number of $(x_1, x_2, ..., x_n)$ which lie in the $i-th$ class. $(y_1, y_2, ..., y_n) \sim Multinomial(n, p_1(\theta), ..., p_k(\theta))$.

$$Q_{k-1} = \sum_{i=1}^{k} \frac{(y_i - np_i(\theta))^2}{np_i(\theta)} \sim \chi^2(k-1).$$

Problems with the above method:

1. k is arbitrary. So, $E(Y_i) = np_i \geq 5$, for asymptotic results to hold true.

2. Formation of classes is arbitrary also. If X is a continuous random variable, then classes of equal probability will take care of the problem mentioned previously.

Example: $H_0 : X \sim N(0,1)$ Find c such that $p_i = P(c_{i-1} < X < c_i) = \frac{1}{k}, k = 1,2,3,....$ For $k = 10$,

c_1	$P(Z < c_1) = 0.1$
c_2	$P(Z < c_2) = 0.2$
c_3	$P(Z < c_3) = 0.3$
.	.
.	.
.	.
c_9	$P(Z < c_9) = 0.9$
c_{10}	$P(Z < c_{10} = \infty$

The classes are $(-\infty, c_1), (c_1, c_2), ..., (c_9, \infty)$.

Example: Use the random number table on page 691 of the text book. $H_0 : X \sim U(0,1)$. $F(x) = 1, 0 < x < 1$. $n = 50, k = 5$ of classes of equal probability.

class:	1	2	3	4	5
Interval:	(0,0.2)	(0.2,0.4)	(0.4,0.6)	(0.6,0.8)	(0.8,1)
p_i	0.2	0.2	0.2	0.2	0.2
Y_i	10	11	10	11	8
np_i	10	10	10	10	10

$$Q_{k-1} = q_4 = \frac{(10-10)^2}{10} + \cdots + \frac{(8-10)^2}{10} = 0.6.$$

$\alpha = 0.05, \chi^2(4) = 9.488$. Since $0.6 < 9.488$, do not reject H_0.

Example: Problem 9.5-5 on page 556 of the text book.

$$H_0 : f(x) = \frac{3}{2}x^2, -1 < x < 1.$$

$$W = \frac{\bar{x}}{\sqrt{\frac{3}{5n}}}.$$

The real null is $H_0 : W \sim N(0,1)$for $n = 7$. Let m be the sample size. Then, $w_1, w_2, ..., w_m, m = 1000$. $k = 19$. The classes are:

A_i	p_i	Y_i	np_i
$(-\infty, -2.55)$	0.0054	3	5.4
$(-2.55, -2.25)$	0.0068	4	6.8
.	.	.	.
.	.	.	.
.	.	.	.
$(2.55, \infty)$	0.0054	5	5.4

$p_i = \frac{1}{19}$ for equal probability classes. $q_{18} = 39.988, \alpha = 0.05, \chi_{0.05}(18) = 28.87$. Since $39.988 > 28.87$, reject H_0.

7.15 More on the Chi Square Goodness of Fit Test

Suppose $X \sim F(x|\theta)$ and θ is unknown this time. Let $\hat{\theta}$ be the minimum Chi-squared estimate that minimizes Q.

$$\hat{Q} = \sum_{i=1}^{n} \frac{[Y-i-np_i(\hat{\theta})]^2}{np_i(\hat{\theta})} \to \chi^2(k-r-1),$$

where r is the number of parameters. If we use the MLE, $\tilde{\theta}$, then

$$\hat{Q} = \sum_{i=1}^{n} \frac{[Y-i-np_i(\tilde{\theta})]^2}{np_i(\tilde{\theta})} \to \chi^2(k-r-1) + W.$$

When you do not reject using $\tilde{Q}$, then you will never reject using $\tilde{Q}$.

Example: Problem 9.5-3 on page 553 of the text book. X is the alpha particles emitted by barium-133. $H_0 : X \sim Poisson(\theta)$. $n = 50$. $f(x|\theta) = \frac{e^{-\theta}\theta^x}{x!}$. $\tilde{\theta} = \bar{x} = 5.4$.

Class	p_i	Y_i	np_i
$A_1 : (0,1,2,3)$	0.213	13	10.65
$A_2 : (4)$	0.160	9	8.0
$A_3 : (5)$	0.173	6	8.65
$A_4 : (6)$	0.156	5	7.83
$A_5 : (7)$	0.120	7	6.00
$A_6 : (8,\infty)$	0.178	10	8.90

$\hat{Q} = \frac{(13-10.65)^2}{10.65} + \cdots + \frac{(10-8.9)^2}{8.9} = 2.763$. $k = 6, r = 1, \chi^2(6-1-1) = 9.488$ Thus, do not reject H_0. How to make classes for H_0 when $H_0 :\sim N(\mu_0, \sigma_0^2)$. If $Z \sim N(0,1)$, then we can find $c_1, c_2, ..., c_{k-1}$, $P(c_{i-1} < z < c_i) = \frac{1}{k}$.

Example: $k = 10$. $P(Z < c_1) = 0.1)$, $P(Z < c_2) = 0.2$, etc.

$$P(x \le d_i) = \frac{i}{k} = P\left(\frac{x-\mu_0}{\sigma_0} < \frac{d_i-\mu_0}{\sigma_0}\right) = P\left(Z < \frac{d_i-\mu_0}{\sigma_0}\right).$$

$\frac{i}{k} = P(Z < c_i)$. Therefore, $c_i = \frac{d_i-\mu_0}{\sigma_0}$. Which leads to $d_i = \mu_0 + \sigma_0 c_i$. The classes are:

Standard Normal	$N(\mu_0, \sigma_0)$
$(-\infty, c_1)$	$(-\infty, d_1)$
(c_1, c_2)	(d_1, d_2)
(c_2, c_3)	(d_2, d_3)
.	.
.	.
.	.
.	.

Example: $H_0 : X \sim Exponential(\theta), \theta = 2$. $x_1, x_2, ..., x_n$ is an iid sequence. Make 10 classes of equal probability. The pdf is given by: $f(x) = \frac{1}{2}e^{-\frac{x}{2}}$. The cdf is given by: $F(x) = 1 - e^{-\frac{x}{2}}$. Find c_i such that $f(c_i) = \frac{i}{10}$.

$$1 - e^{-\frac{c_i}{2}} = \frac{i}{10} \Rightarrow -\frac{c_i}{2} = \log\left(1 - \frac{i}{10}\right) \Rightarrow c_i = -2\log\left(1 - \frac{i}{10}\right).$$

7.16 Comparison of Two Multinomials

Example: Compare the grade distribution of male and female students.

Class:	1	2	...	i	...	k	Total
	y_{11}	y_{21}	...	y_{i1}	...	y_{k1}	n_1
	p_{11}	p_{21}	...	p_{i1}	...	p_{k1}	
	y_{12}	y_{22}	...	y_{i2}	...	y_{k2}	n_2
	p_{12}	p_{22}	...	p_{i2}	...	p_{k2}	

The probabilities must be the same for both classes. n_1 and n_2 can be different. $H_0 : p_{i1} = p_{i2} = p_i, i = 1, 2, ..., k$. For the first sample, the test statistic is,

$$\sum_{i=1}^{k} \frac{(y_{i1} - n_1 p_{i1})^2}{n_1 p_{i1}} \to \chi^2(k-1).$$

For the second sample, the test statistic is,

$$\sum_{i=1}^{k} \frac{(y_{i2} - n_2 p_{i2})^2}{n_2 p_{i2}} \to \chi^2(k-1).$$

For the combined sample, the test statistic is,

$$\sum_{j=1}^{2}\sum_{i=1}^{k} \frac{(y_{ij} - n_j p_{ij})^2}{n_j p_{ij}} \to \chi^2(2(k-1)).$$

$$\hat{p}_i = \frac{y_{i1} + y_{i2}}{n_1 + n_2}, i = 1, 2, ..., k, \ \hat{Q} = \sum_{j=1}^{2}\sum_{i=1}^{k} \frac{(y_{ij} - n_j \hat{p}_{ij})^2}{n_j \hat{p}_{ij}} \to \chi^2(k-1).$$

Example: Problem 9.6-1 on page 563 of the text book.

						Total
Grade:	A	B	C	D	F	
Class:	1	2	3	4	5	
Group I:	8	13	16	10	3	50
Group II:	4	9	14	16	7	50
$\hat{p}_i$	0.12	0.22	0.30	0.26	0.10	

$$\hat{Q}_1 = \frac{(8 - 50(0.12))^2}{50(0.12)} + \cdots + \frac{(3 - 50(0.10))^2}{50(0.10)}, \ \hat{Q}_2 = \frac{(4 - 50(0.12))^2}{50(0.12)} + \cdots + \frac{(7 - 50(0.10))^2}{50(0.10)},$$

$\hat{Q}_1 + \hat{Q}_2 = 5.18$. $\chi^2_{0.05}(4) = 9.488$. Thus, the grade distributions are the same.

7.17 Comparison of Several Multinomials

Example: Compare grade distributions for the graduating classes in 1990, 1991, 1992, 1993, 1994, and 1995. $y_{ij}, i = 1, 2, ..., k, j = 1, 2, ..., h$. $H_0 : p_{ih} = p_i, i = 1, 2, ..., k; j = 1, 2, ..., h$.

$$\sum_{j=1}^{h}\sum_{i=1}^{k} \frac{(y_{ij} - n_j\hat{p}_i)^2}{n_j p_i} \to \chi^2[(h-1)(k-1)], \ \hat{p}_i = \frac{1}{n}\sum_{j=1}^{h} y_{ij}, n = n_1 + n_2 + \cdots + n_h.$$

7.18 Contingency Tables

Example: There are n people. Classify according to education and income. The question to be answered is, are income levels and education dependent or independent?

Classify according to two attributes. Test if the attributes are independent. Suppose attribute B has h levels and attribute A has k levels. Then,

	B_1	B_2	...	B_j	...	B_h	
A_1	y_{11}	y_{12}	...	y_{1j}	...	y_{1h}	$p_{1\cdot}$
A_2	y_{21}	y_{22}	...	y_{2j}	...	y_{2h}	$p_{2\cdot}$
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
A_i	y_{i1}	y_{i2}	...	y_{ij}	...	y_{ih}	$p_{i\cdot}$
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.
	$p_{\cdot 1}$	$p_{\cdot 2}$	...	$p_{\cdot j}$	...	$p_{\cdot h}$	n

$p_{ij} = P(\text{subject lies in (i,j)-th cell}) = P(\text{subject belongs to } A_i, B_j)$. y_{ij} is the number of subjects in the $(i, j) - th$ cell. $p_{i\cdot} = \sum_{j=1}^{h} p_{ij} = P(A_i)$. $p_{\cdot j} = \sum_{i=1}^{k} p_{ij} = P(B_j)$. $H_0 : p_{ij} = p_{i\cdot}p_{\cdot j}$. That is, the two attributes are independent.

$$\sum_{i=1}^{h}\sum_{j=1}^{k} \frac{(y_{ij} - np_{ij})^2}{np_{ij}} \to \chi^2(hk-1), \ \sum_{i=1}^{h}\sum_{j=1}^{k} \frac{(y_{ij} - np_{i\cdot}p_{\cdot j})^2}{np_{i\cdot}p_{\cdot j}} \to \chi^2(hk-1), \ \hat{p}_{i\cdot} = \frac{Y_{i\cdot}}{n}, \ \hat{p}_{\cdot j} = \frac{Y_{\cdot j}}{n},$$

The test statistic is:

$$\hat{Q} = \sum_{i=1}^{h}\sum_{j=1}^{k} \frac{(y_{ij} - n\hat{p}_{i\cdot}\hat{p}_{\cdot j})^2}{n\hat{p}_{i\cdot}\hat{p}_{\cdot j}} \to \chi^2((h-1)(k-1)).$$

Reject H_0 if $\hat{Q} > \chi^2((h-1)(k-1))$. $E(Y_{ij}) = np_{ij} = np_{i\cdot}p_{\cdot j}$ if H_0 is true.

Example: A sample of 1000 smokers and non-smokers and cancer(yes/no).

	Smoker	Non-smoker	
Yes	30(15)	20(35)	50
No	270(285)	680(665)	950
	300	700	1000

$\hat{p}_{1\cdot} = 0.05, \hat{p}_{2\cdot} = 0.95$. $\hat{p}_{\cdot 1} = 0.30, \hat{p}_{\cdot 2} = 0.70$. $E(Y_{ij}) = np_{i\cdot}p_{\cdot j} = n\frac{Y_{i\cdot}}{n}\frac{Y_{\cdot j}}{n} = \frac{1}{n}Y_{i\cdot}Y_{\cdot j}$. $\hat{Q} = \frac{(30-15)^2}{15} + \frac{(20-35)^2}{35} + \frac{(270-285)^2}{285} + \frac{(680-665)^2}{665} = 22.56$. $\chi^2(1) = 6.635$. Since $22.56 > 6.635$, the variables are dependent. $P(cancer|smoker) = \frac{30}{300} = 0.1$. $P(cancer|non-smoker) = \frac{20}{700} = 0.029$. Thus, you are 3-1/2 times more likely to get cancer if you smoke.

7.19 Non-parametric Methods

$x \sim f(x|\theta)$; Up till now, we assumed some distribution for X which involves parameters. For the remaining sections, do not assume any distribution. We will do some statistical analysis without the distribution of X. $x_1, x_2, ..., x_n$ is an *ordered sample* if y_1 is the smallest and y_2 is the second to the smallest on up to y_n being the largest. $y_1 < y_2 < ... < y_n$. Assume that X is a continuous random variable. No two y's are the same. Find the distribution of Y_r. X has a cdf $F(x)$. $F(x) = P(X \leq x)$. $P(Y_r \leq y)$. Let $T = (\#(x_1, x_2, ..., x_n) \leq y)$. Then, $T \sim Binomial(n, p), p = F(y)$.

$$P(Y_r \leq y) = P(T \geq r) = G_x(y) = \sum_{t=r}^{n} \binom{n}{t} F^t(y)(1 - f(t))^{n-r}.$$

$$g_r(y) = \frac{\partial G_r(y)}{\partial y} = \frac{n!}{(r-1)!(n-r)!}F(y)^{r-1}[1 - F(y)]^{n-r}f(y).$$

The pdf of y_1 is $g_1(y) = n[1 - F(y)]^{n-1}f(y)$. The pdf of y_n is $g_n(y) = nF(y)^{n-1}f(y)$.

Example: Suppose that $X \sim Uniform(0, \theta)$. $x_1, x_2, ..., x_n$ is an iid sequence. $\hat{\theta} = x_{\max} = Y_n$. $E(\hat{\theta}) = E(Y_n)$. $f(x) = \frac{1}{\theta}, 0 < x < \theta$.

$$F(x) = \int_0^x \frac{1}{\theta}\, dx = \frac{x}{\theta}.$$

Then,

$$g_n(y) = nF(y)^{n-1}f(y) = n\left(\frac{y}{\theta}\right)^{n-1}\frac{1}{\theta} = \frac{ny^{n-1}}{\theta^n}, 0 < y < \theta.$$

$$E(Y_n) = \int_0^\theta y g_n(y)\, dy = \frac{n}{\theta^n}\int_0^\theta y^n\, dy = \frac{n}{\theta^n}\frac{y^{n+1}}{n+1}\bigg|_0^\theta = \frac{n\theta}{n+1},$$

which is biased. $\tilde{\theta} = \frac{(n+1)\theta}{n}$ is an unbiased estimator. So to find $g_{10} : g_{10}(y) = \frac{10y^9}{\theta^{10}}$.

Example: Suppose a size of 5 from $U(0, 1)$. Find $P\left(\frac{1}{3} < Y_3 < \frac{2}{3}\right)$. $n = 5$, $g_3(y) = \frac{5!}{2!2!}F(y)^2[1 - F(y)]^2 f(y)$. From the uniform distribution we get $f(x) = 1; F(x) = x$. So, $g_3(y) = 30y^2(1 - y^2)1, 0 < y < 1$.

$$P\left(\frac{1}{3} < Y_3 < \frac{2}{3}\right) = \int_{\frac{1}{3}}^{\frac{2}{3}} 30y^2(1 - y^2)\, dy = \frac{30y^3}{3} - \frac{30y^5}{5}\bigg|_{\frac{1}{3}}^{\frac{2}{3}} = 0.58.$$

What is the $P\left(\frac{1}{3} < x < \frac{2}{3}\right)$? $\frac{2}{3} - \frac{1}{3} = \frac{1}{3}$. The order statistic will be used to find the confidence interval of the median(not the mean).

7.19.1 Estimation of $\prod_p$

$\prod p = 100p - th$ percentile of the distribution. $p = P(X \leq \prod_p)$, $x_1, x_2, ..., x_n$ is an iid sequence. $Y_1, Y_2, ..., Y_n$ is the ordered set. $F(x) = P(X \leq x)$. For any continuous random variable, the transformation is $Y = F(x)$.

Then, $Y \sim U(0,1)$. $F(x_1), F(x_2), ..., F(x_n)$ is an ordered sample from $U(0,1)$. $W_i = F(Y_i), i = 1, 2, ..., n$. $W_1, W_2, ..., W_n$ is an ordered sample from $U(0,1)$. The distribution of W_r is

$$g_r(W) = \frac{n!}{(r-n)!(n-r)!} W^{r-1}(1-W)^{n-r}, 0 < W < 1.$$

Then,

$$\int_0^1 W^{r-1}(1-W)^{n-r}\,dw = \frac{(r-1)!(n-r)!}{n!}.$$

$$E(W_r) = \int_0^1 W g_r(W)\,dw = \frac{n!}{(r-1)!(n-r)!}\int_0^1 W^r(1-W)^{n-r}\,dw =$$

$$\frac{n!}{(r-n)!(n-r)!}\frac{r!(n-r)!}{(n-r+r+1)!} = \frac{r}{n+1}.$$

$E(W_r - W_{r-1}) = \frac{1}{n+1}$. The above equation holds true for any distribution shape. Find r such that $E(F(Y_r)) = W(W_r) = p$. $r = p(n+1)$. Y_r is an estimator of $\prod p$ if $r = p(n+1)$. Interpolate between two integers nearest $p(n+1)$ if $p(n+1)$ is not an integer.

Example: $n = 31$, estimate the median of X. $m = \prod_{\frac{1}{2}}$ or $P(X < m) = \frac{1}{2}$. $r = 32(\frac{1}{2}) = 16$. $\hat{m} = Y_{16}$.

Example: $n = 8$. The following is an ordered sample.

i	1	2	3	4	5	6	7	8
Y_i	2.4	2.8	2.9	3.1	3.5	3.9	4.0	4.2

Estimate $\prod_{\frac{1}{4}}$ and $\prod_{\frac{1}{2}}$. From $\prod_{\frac{1}{4}}$ $p = \frac{1}{2}$. Thus, $r = \frac{9}{4} = 2.25$. Since $2 < 2.25 < 3$,

$$\hat{\prod}_{\frac{1}{4}} = \frac{3}{4}Y_2 + \frac{1}{4}Y_3 = 2.825,\ \prod_{\frac{1}{2}} = \frac{9}{2} = 4.5,\ \hat{\prod}_{\frac{1}{2}} = \frac{Y_4 + Y_5}{2} = \frac{3.1 + 3.5}{2} = 3.3.$$

7.19.2 Confidence Intervals for $\prod_p$

$T = \#(x_1, x_2, ..., x_n) < \prod_p$. $T \sim Binomial(n, f(\prod_p) = p)$. (Y_i, Y_j) is the confidence interval of $\prod_p$. What is the level of this interval?

$$P(Y_i < \prod_p < Y_j) = P(i \le T \le j-1) = \sum_{k=i}^{j-1} \left(\begin{array}{c} n \\ k \end{array}\right) p^j q^{n-k}.$$

How do we choose (i, j) so that (Y_i, Y_j) is the confidence interval of $\prod_p$ with a given level of confidence?

Example: $n = 19$. Find the confidence interval of $\prod_{\frac{1}{4}}$. The point estimate of $\prod_{\frac{1}{4}}$ is $(n+1)p = \frac{20}{4} = 5$. Thus, Y_5 is a point estimate of $\prod_{\frac{1}{4}}$. $i = r - k$ and $j = r + k, k = 1, 2, ...$

Example: For a given sample of size 12, what is the confidence level of (Y_4, Y_{10}) as a confidence interval for the median? $m = \prod_{\frac{1}{2}}$. $P(Y_4 < \prod_{\frac{1}{2}} < Y_{10}) =$

$$P(4 \le T \le 9) = \sum_{k=4}^{9} \left(\begin{array}{c} 12 \\ k \end{array}\right) \left(\frac{1}{2}\right)^{12} = 0.9077.$$

Find (i,j) for the confidence interval of $\prod_{\frac{1}{2}}$. $r=(n+1)p=\frac{n+1}{2}$. Thus,

$$\left(\frac{n+1}{2}-i\right)=\left(j-\frac{n+1}{2}\right).$$

Use Table 10.2-1 on page 602 of the text book. For large n, the confidence interval of $\prod_p$ is derived as follow: Find (i,j) such that $P(Y_i<\prod_p<Y_j)=P(i\le T\le j-1)$, $T\sim Binomial(n,p)$. $\frac{T-np}{\sqrt{npq}}\to N(0,1)$. So,

$$P(i-0.5\le T\le j-1+0.5)=P(i-0.5\le T\le j-0.5)=P\left(\frac{i-0.5-np}{\sqrt{npq}}\le z\le\frac{j-0.5-np}{\sqrt{npq}}\right)=1-\alpha,$$

$1-\alpha=P(-z_{\alpha/2}\le z\le z_{\alpha/2})$. To find i and j : $\frac{i-0.5-np}{\sqrt{npq}}=-z_{\alpha/2}$, $i=np+0.5-z_{\alpha/2}\sqrt{npq}$. $j=np+0.5+z_{\alpha/2}\sqrt{npq}$.

7.19.3 Homework

9.1-2 $n=100, x_1=30, x_2=35, x_3=15$. $n-x_1-x_2-x_3=20$. Since $f(x_1,x_2,x_3,x_4)\ne f_1(x_1)f_2(x_2)f_3(x_3)f_4(x_4)$, the distribution is hypergeometric.

(a) $$f(x_1,x_2,x_3)=\frac{\binom{30}{x_1}\binom{35}{x_2}\binom{15}{x_3}\binom{20}{15-x_1-x_2-x_3}}{\binom{100}{15}}$$

(b) Non-negative integers (x_1,x_2,x_3) such that $x_1+x_2+x_3\le 15$.

(c) $$f_1(x_1)=\frac{\binom{30}{x_1}\binom{70}{15-x_1}}{\binom{100}{15}},\quad P_1(x_1=10)=\frac{\binom{30}{10}\binom{70}{5}}{\binom{100}{15}}=0.001435373.$$

(d) $$f_{12}(x_1,x_2)=\frac{\binom{30}{x_1}\binom{35}{x_2}\binom{35}{15-x_1-x_2}}{\binom{100}{15}}$$

9.1-16: $f(x,y)=2, 0\le y\le x\le 1$.

(a) The marginal pdf of x is

$$f_1(x)=\int_0^x f(x,y)\,dy=\int_0^x 2\,dy=2x, 0\le x\le 1.$$

The marginal pdf of y is

$$f_2(y)=\int_y^1 f(x,y)\,dx=\int_y^1 2\,dx=2(1-y), 0\le y\le 1.$$

(b)

$$\mu_x=\int_0^1 xf_1(x)\,dx=\int_0^1 2x^2\,dx=\frac{2}{3},\quad \mu_y=\int_0^1 yf_2(y)\,dy=\int_0^1 2y-2y^2\,dy=\frac{1}{3}.$$

$$\sigma_x^2=\int_0^1 x^2f_1(x)-\mu_x^2\,dx=\int_0^1 2x^3-\mu_x^2\,dx=\frac{1}{2}-\frac{4}{9}=\frac{1}{18}.$$

$$\sigma_y^2 = \int_0^1 y^2 f_2(y) - \mu_y \, dy = \int_0^1 2y^2 - 2y^3 - \mu_y^2 \, dy = \frac{2}{3} - \frac{1}{2} = \frac{1}{18}.$$

$$Cov(x,y) = \int_0^1 \int_y^1 2xy - \mu_x \mu_y \, dx \, dy = \frac{1}{36}, \quad \rho = \frac{Cov(x,y)}{\sigma_x \sigma_y} = \frac{\frac{1}{36}}{\sqrt{\frac{1}{18}\frac{1}{18}}} = \frac{1}{2}.$$

(c) $E(Y|x) = \int_0^x y h(Y|x) \, dy = \int_0^x \frac{y}{x} \, dy = \frac{x}{2}$. The regression line is $Y = \frac{x}{2}$. The line makes sense because the least squares line is below the 45° line. The upper bound on y is x.

9.2-1: $f(x,y) = \frac{x+y}{32}, x = 1,2; y = 1,2,3,4.$

(a)

$$f(1,1) = \frac{1}{16};\ f(1,2) = \frac{3}{32};\ f(1,3) = \frac{1}{8};\ f(1,4) = \frac{5}{32}.$$

$$f(2,1) = \frac{3}{32};\ f(2,2) = \frac{1}{8};\ f(2,3) = \frac{5}{32};\ f(2,4) = \frac{3}{16}.$$

$$f_1(x) = \sum_{y=1}^{4} \frac{x+y}{32} = \frac{2x+5}{16}, \quad f_2(y) = \sum_{x=1}^{2} \frac{x+y}{32} = \frac{3+2y}{32}.$$

(b) $g(x|y) = \frac{f(x,y)}{f_2(y)} = \frac{x+y}{3+2y}$.

(c) $h(y|x) = \frac{f(x,y)}{f_1(x)} = \frac{x+y}{4x+10}$.

(d) $P(1 \le Y \le 3|x=1) = \sum_{y=1}^{3} \frac{x+y}{4x+10} = \sum_{y=1}^{3} \frac{1+Y}{14} = \frac{2}{14} + \frac{3}{14} + \frac{4}{14} = \frac{9}{14}$. $P(Y \le 2|x=2) = \sum_{y=1}^{2} \frac{2+y}{18} = \frac{3}{18} + \frac{4}{18} = \frac{7}{18}$, $P(x=2|y=3) = \sum_{x=2}^{2} \frac{x+3}{9} = \frac{2+3}{9} = \frac{5}{9}$.

(e) $E(Y|x=1) = \sum_{y=1}^{4} y h(Y|x) = \sum_{y=1}^{4} y \left(\frac{1+y}{14}\right) = \sum_{y=1}^{4} \frac{y+y^2}{14} = \frac{2}{14} + \frac{2+4}{14} + \frac{3+9}{14} + \frac{4+16}{14} = \frac{20}{7}$. $Var(Y|x=1) = \sum_{y=1}^{4} \left[y - \frac{20}{7}\right] h(Y|x) = \sum_{y=1}^{4} \left[y - \frac{20}{7}\right] \left[\frac{1+y}{14}\right] = \frac{55}{49}$.

9.2-10 $f_1(x) = \frac{1}{10}, x = 0,1,2,...,9$. $h(Y|x) = \frac{1}{10-x}, y = x, x+1, ...9$.

(a) $f(x,y) = f_1(x) h(Y|x) = \frac{1}{10}\left[\frac{1}{10-x}\right] = \frac{1}{100-10x}$.

(b) $f_2(y) = \sum_{x=0}^{y} f(x,y)$....

(c) $E(Y|x) = \sum_{y=x}^{9} y h(Y|x) = \sum_{y=x}^{9} \frac{y}{10-x} = \frac{9(10-x) - \frac{(9-x)(10-x)}{2}}{10-x}, x \in 0,1,...,9.$

9.3-5 $X, Y \sim BivariateNormal$. $\mu_x = 185; \mu_y = 84; \sigma_x^2 = 100; \sigma_y^2 = 64; \rho = \frac{3}{5}$.

(a)

$$N\left[84 + \frac{3}{5}\sqrt{\frac{64}{100}}(190-185), 64\left(1 - \frac{9}{25}\right)\right] = N(86.4, 40.96].$$

(b)

$$P(86.4 < y < 95.36|x=190) = P\left(\frac{86.4-86.4}{\sqrt{40,96}} < \frac{Y-86.4}{\sqrt{40.96}} < \frac{95.36-86.4}{\sqrt{40.96}}\right) =$$

$$P\left(0 < \frac{Y-86.4}{\sqrt{40.96}} < 1.4\right) = \Phi(1.4) - \Phi(0) = 0.9192 - 0.5 = 0.4192.$$

9.4-2

$$S_{xy} = \frac{1}{5}\sum_{i=1}^{6}(x_i - \bar{x})(y_i - \bar{y}) = -\frac{475}{5} = -95.$$

$\bar{x} = 184.6667;\ \bar{y} = 176.5.$

$$S_x = \sqrt{\frac{1}{5}\sum_{i=1}^{6}(x_i - \bar{x})^2} = 10.3086,\ S_y = \sqrt{\frac{1}{5}\sum_{i=1}^{6}(y_i - \bar{y})^2} = 22.3137.$$

$$R = \frac{S_{xy}}{S_x S_y} = \frac{-95}{(10.3086)(22.3137)} = -0.413002,\ T = \frac{R\sqrt{n-2}}{\sqrt{1-R^2}} = \frac{-0.413002\sqrt{4}}{\sqrt{1-(-0.413002)^2}} = -0.90697.$$

$H_0 : \rho = 0$. $H_1 : \rho \neq 0$. $\alpha = 0.10; t_{0.05}(4) = 2.132$. Since $|-0.90697| < 2.132$, do not reject H_0.

9.5-5 $n = 432.$

	Y_i	p_i	np_i
Red-eyed	254	$\frac{9}{16}$	243
Brown-eyed	69	$\frac{3}{16}$	81
Scarlet-eyed	87	$\frac{3}{16}$	81
White-eyed	22	$\frac{1}{16}$	27

$q_3 = \sum_{i=1}^{4}\frac{(y_i - np_i)^2}{np_i} = \frac{11^2}{243} + \frac{(-12)^2}{81} + \frac{6^2}{81} + \frac{(-5)^2}{27} = 3.6461$. $\chi^2_{0.05}(3) = 7.815$. Since $3.6461 < 7.815$, the null hypothesis is not rejected.

9.5-13 $\bar{x} = 42.4.$

Category	Frequency	Probability
(0,7.55)	15	0.163
(7.55,16.1)	12	0.153
(16.1,24.65)	11	0.125
(24.65,33.2)	9	0.102
(33.2,41.75)	8	0.083
(41.75,50.3)	6	0.068
(50.3,58.85)	8	0.056
(58.85,75.95)	7	0.076
(75.95,101.6)	8	0.076
(101.6,∞)	6	0.091

$\sum_{i=1}^{10}\frac{(y_i - np_i)}{np_i} = 2.83429517$. This does not match the STATGRAPHICS printout nor the author's answer because they probably used the true mean of $\bar{x} = 42.2$.

9.6-13

$\hat{p}_{1\cdot} = 0.25; \hat{p}_{2\cdot} = 0.397; \hat{p}_{3\cdot} = 0.353.$

$\hat{p}_{\cdot 1} = 0.485; \hat{p}_{\cdot 2} = 0.423; \hat{p}_{\cdot 3} = 0.092.$

The expected values are:

1004(0.25)(0.485)	121.735
1004(0.25)(0.423)	106.173
1004(0.25)(0.092)	23.092
1004(0.397)(0.485)	193.32
1004(0.397)(0.423)	168.603
1004(0.397)(0.092)	36.67
1004(0.353)(0.485)	171.89
1004(0.353)(0.423)	149.92
1004(0.353)(0.092)	32.61

$q = \frac{(128-121.735)^2}{121.735} + \cdots + \frac{(36-32.61)^2}{32.61} = 10.064$. $\chi^2_{0.05}(4) = 9.488, \chi^2_{0.025}(4) = 11.14$. $0.025 < p < 0.05$.

9.6-14 **(a)**

	News	TV	Radio	Totals
Under 35	30(47.48)	68(47.73)	10(12.81)	108
35-54	61(70.33)	79(70.70)	20(18.98)	160
Over 54	98(71.20)	43(71.57)	21(19.21)	162
Totals	189($\hat{p}_{\cdot 1} = 0.4395$)	190		
	51	430		

$\hat{Q} = \frac{(30-47.48)^2}{47.48} + \cdots + \frac{(21-19.21)^2}{19.21} = 38.67$. $\chi^2_{0.05}(2(2)) = 9.488$. Since $38.67 > 9.488$, reject H_0. Media credibility and age are dependent.

(b)

	News	TV	Radio	Totals
Male	92(96.39)	108(96.39)	19(26.01)	219
Female	97(92.61)	81(92.61)	32(24.99)	210
Totals	189($\hat{p}_{\cdot 1} = 0.44$)	189	51($\hat{p}_{\cdot 3} = 0.12$)	429

$\hat{Q} = \frac{(92-96.39)^2}{96.39} + \cdots + \frac{(32-24.99)^2}{24.99} = 7.12$. $\chi^2_{0.05}(2(1)) = 5.991$. Since $7.12 > 5.991$, reject H_0. Media credibility an sex are dependent.

(c)

	News	TV	Radio	Totals
Grade School	45(31.96)	22(32.13)	6(8.33)	73
High School	94(105.28)	115(105.84)	30(27.44)	239
College	49(50.76)	52(51.03)	13(13.23)	114
Totals	188($\hat{p}_{\cdot 1} = 0.44$	189	49	426

$\hat{Q} = \frac{(45-31.96)^2}{31.96} + \cdots + \frac{(13-13.23)^2}{13.23} = 11.49$. $\chi^2_{0.05}(2(2)) = 9.488$. Since $11.49 > 9.488$, reject H_0.

(d) The $p-$value for (a) is $p < 0.01$, for (b), $0.025 < p < 0.05$, for (c), $0.01 < p < 0.025$.

7.19.4 Testing about the Median

The *Binomial Test(sign test)* will be presented. $H_0 : m = m_0$. $H_1 : m < m_0$. $x_1, x_2, ..., x_n$ is an iid sequence. Look at $x_1 - m_0, x_2 - m_0, ..., x_n - m_0$. Y is the number of negative signs in $x_i - m_0$. $Y \sim Binomial(n, p)$. $H_0 : p = \frac{1}{2}$. $H_1 : p > \frac{1}{2}$. Reject H_0 if $Y \geq c$.

$$\alpha = P(\text{Reject } H_0|H_0) = P(Y \geq c|p = \frac{1}{2}) = \sum_{y=c}^{n} \left(\begin{array}{c} n \\ y \end{array} \right) \left(\frac{1}{2}\right)^n.$$

$$K(p) = P(\text{Reject } H_0|H_1) = P(Y \geq c|p) = \sum_{y=c}^{n} \binom{n}{y} p^y q^{n-y}.$$

How to find c for large n :

$$\alpha = P(Y \geq c|p = \frac{1}{2}) = P(Y \geq c - \frac{1}{2}|p = \frac{1}{2}) = P\left(\frac{Y - \frac{n}{2}}{\sqrt{\frac{n}{4}}} \geq \frac{c - \frac{1}{2} - \frac{n}{2}}{\sqrt{\frac{n}{4}}}\right) =$$

$$P\left(z \geq \frac{c - \frac{1}{2} - \frac{n}{2}}{\sqrt{\frac{n}{4}}}\right) = \alpha = P(Z \geq z_\alpha).$$

$$\frac{c - \frac{1}{2} - \frac{n}{2}}{\sqrt{\frac{n}{4}}} = z_\alpha \Rightarrow c = \frac{n}{2} + \frac{1}{2} + \frac{z_\alpha \sqrt{n}}{2}.$$

Example: Problem on page 608 of the text book. X is the length of a fish. $H_0 : m = 3.7$. $H_1 : m > 3.7$. $H_0 : p = \frac{1}{2}$. $H_1 : p < \frac{1}{2}$. Let y be the number of fish ≤ 3.7. Reject Y if $Y \leq c$ for $\alpha = 0.0547$. $n = 10, c = 2$.

$$0.0547 = \sum_{y=0}^{2} \binom{10}{y} \left(\frac{1}{2}\right)^{10}.$$

The given sample is 5.0,3.9,5.2,5.5,2.8,6.1,6.4,2.6,1.7,4.3. Since $Y = 3$, do not reject H_0.

7.19.5 Testing for $\prod_p$ for a Fixed p

$H_0 : \prod_p = a$, $H_1 : \prod_p > a$. Y is the number of $(x_1, x_2, ..., x_n) \leq a$. $Y \sim Binomial(n, p^*)$. $H_0 : p^* = p$. $H_1 : p^* < p$. The bivariate sample is $(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)$. Test if $p = P(X > Y) = \frac{1}{2}$. If so, then $P(X < Y) = \frac{1}{2}$. Test to see if X and Y have the same median. $W_i = X_i - Y_i$, $w_1, w_2, ..., w_n$. Suppose $m = median(W)$. Then, $H_0 : m = 0$. $H_1 : m > 0$. The weakness of the sign test is given in the following diagram:

7.19.6 Wilcoxon Test for Median

Let $m = median(X)$. Suppose the distribution is symmetric about the median. Then, $H_0 : m = m_0$. $H_1 : m > m_0$. $x_1, x_2, ..., x_n$ is an iid sequence. $x_1 - m_0, x_2 - m_0, ..., x_n - m_0$.

$$U_i = \begin{cases} -1, & \text{if } x_i - m_0 < 0. \\ 1, & \text{if } x_i - m_0 > 0. \end{cases}$$

R_i is the rank of $|x_i - m_0|$. U_i and R_i are independent. $W = \sum_{i=1}^{n} U_i R_i$, which is the sum of the ranks of positive $x_i - m_0$ minus negative $x_i - m_0$. If H_0 is true, then $E(W) = 0; Var(W) = \frac{n(n+1)(2n+1)}{6} = \sigma_w^2$. $z = \frac{W-0}{\sigma_w} \sim N(0, 1)$, for large n. Reject H_0 if $z > z_\alpha$. If $H_1 : w < w_0$, then reject H_0 if $z < -z_\alpha$.

U_i	p
-1	$\frac{1}{2}$
1	$\frac{1}{2}$

$E(U_i) = 0, Var(U_i) = 1 = E(U_i^2)$. If r_i is the rank then:

r_i	p
1	$\frac{1}{n}$
2	$\frac{1}{n}$
3	$\frac{1}{n}$
.	.
.	.
.	.
n	$\frac{1}{n}$

$$E(R_i) = \sum_{j=1}^{n} j\left(\frac{1}{n}\right) = \frac{n(n+1)}{2n} = \frac{n+1}{2}.$$

$$Var(R_i) = E(R_i^2) = \sum_{j=1}^{n} j^2\left(\frac{1}{n}\right) = \frac{1}{n}(1^2+2^2+\cdots+n^2) = \frac{n(n+1)(2n+1)}{6n} = \frac{(n+1)(2n+1)}{6}.$$

$$E(W) = \sum_{i=1}^{n} E(U_i)E(R_i) = 0.$$

$$Var(W) = E(W^2) = E\left[\sum_{i=1}^{n} U_i^2 R_i^2 + \sum_{i=1}^{n}\sum_{j=1}^{n} \overbrace{U_iU_j}^{\text{indepnt}}\ \overbrace{R_iR_j}^{\text{depnt}}\right] =$$

$$\sum_{i=1}^{n} E(U_i^2)E(R_i^2) = \sum_{i=1}^{n} \frac{(n+1)(2n+1)}{6} = \frac{n(n+1)(2n+1)}{6}.$$

R_i is the rank of $|x_i - m_0|$. $W = \sum_{i=1}^{n} U_i R_i$. $z = \frac{W-0}{\sigma_w}$. $\sigma_w^2 = \frac{n(n+1)(2n+1)}{6}$.

Example: Problem 10.4-1 on page 615 of the text book. X is the length of swordfish. $H_0 : m = 3.7$. $H_1 : m < 3.7$.

$x_i - m_0$	1.3	0.2	1.5	1.8	-0.9	2.4	2.7	-1.1	-2	0.6
U_i	1	1	1	1	-1	1	1	-1	-1	1
R_i	5	1	6	7	3	9	10	4	8	2

$W = \sum_{i=1}^{10} U_i R_i = 25$. $\sigma_w = 48.06$. $z = \frac{25}{48.06} = 0.58$. Do not reject H_0.

7.19.7 Two Sample Median Test

Given $x_1, x_2, ..., x_n$ and $y_1, y_2, ..., y_n$. $H_0 : m_x = m_y$. Let $\hat{m}$ be the sample median for the combined samples. If $n_1 + n_2 = 2k$, then k of the $n_1 + n_2$ observations are below the median $\hat{m}$. Even if $n_1 + n_2 = 2k + 1$, k of the $n_1 + n_2$ observations are below $\hat{m}$. V is the number of $x_i's$ less than $\hat{m}$.

$$P(V = v) = \frac{\begin{pmatrix} n_1 \\ v \end{pmatrix}\begin{pmatrix} n_2 \\ k-v \end{pmatrix}}{\begin{pmatrix} n_1+n_2 \\ k \end{pmatrix}}, v = 0, 1, ..., \min(n_1, k).$$

H_1	Reject
$m_x < m_y$	$v \geq c$
$m_x > m_y$	$v \leq c$
$m_x \neq m_y$	$v \leq c_1$ or $v \geq c_2$

Example: Problem 10.5-1 on page 623 of the text book. $H_0 : m_x = m_y$. $H_1 : m_x < m_y$. $n_1 = 8, n_2 = 8$. $v = 6$. Reject if $6 \geq c$. Find c. The steps to solve the problem are as follow:

1. Combine the sample.
2. Find the median.
3. Count the number of observations below the median.

Find $p \geq P(v \geq 6)$,

$$P(v = 6) = \frac{\begin{pmatrix} 8 \\ 6 \end{pmatrix}\begin{pmatrix} 8 \\ 2 \end{pmatrix}}{\begin{pmatrix} 16 \\ 8 \end{pmatrix}} = \frac{1}{12870}, \quad P(v = 7) = \frac{67}{12870}, \quad P(v = 8) = \frac{784}{12870}.$$

Therefore, $p = P(v \geq 6) = 0.066$. Given $\alpha = 0.05$, do not reject H_0.

Example: Order the 2 samples together. $x_4, y_1, x_3, x_2 | y_2, y_3, x_1, y_4$. $n_1 = n_2 = 4$. 3 $x's$ fall below the median. So, $v = 3$.

7.19.8 Wilcoxon Two Sample Test

$x_1, x_2, ..., x_n$ and $y_1, y_2, ..., y_n$ are two random samples. $H_0 : m_x = m_y$. Combine both samples and rank all the $(n_1 + n_2)$ observations from 1 to $n_1 + n_2$. W is the sum of ranks or $(y_1, y_2, ..., y_n)$. $r_i = Rank(Y_i)$.

Y_i	$P(Y_i)$
1	$\frac{1}{n_1+n_2}$
2	$\frac{1}{n_1+n_2}$
3	$\frac{1}{n_1+n_2}$
.	.
.	.
.	.
$n_1 + n_2$	$\frac{1}{n_1+n_2}$

$E(R_i) = \frac{n_1+n_2+1}{2}$. $W = R_1 + R_2 + ... + R_{n_2}$. $E(W) = n_2 E(R_i) = n_2 \frac{(n_1+n_2+1)}{2}$. Find $Var(W)$. We need $E(R_i^2)$ and $E(R_i R_j)$. $\sigma_w^2 = n_1 n_2 \frac{(n_1+n_2+1)}{12}$. The variance does not change as $x's$ and $y's$ change. So, $Var(U) = Var(W)$. $z = \frac{W - \mu_w}{\sigma_w}$.

H_1	Reject if
$m_x > m_y$	$z < -z_\alpha$
$m_x < m_y$	$z > z_\alpha$
$m_x \neq m_y$	$\lvert z \rvert > z_{\alpha/2}$

Example: Use the data from problem 10.5-3 on page 627 of the text book. $n_1 = n_2 = 8$. $H_0 : m_x = m_y$. $H_1 : m_x < m_y$. The ranks of Y are 3, 8, 9, 11, 12, 13, 15, 16. Only the first two fall below the combined median. $W = 3 + 8 + 9 + \cdots + 16 = 87$. $\mu_w = 8\left(\frac{17}{2}\right) = 68$. $\sigma_w = 9.52$. $z = \frac{87-68}{9.52} = 1.996$. Since $1.996 > z_{0.05} = 1.64$, reject H_0.

7.19.9 Run Test

$X \sim F(x)$, $Y \sim F(y)$. $F(x) = P(X \leq x)$. $H_0 : F(z) = G(z), \forall z$. $H_1 : F(z) \neq G(z)$. $x_1, x_2, ..., x_n$ and $y_1, y_2, ..., y_n$ are two iid samples. Order the $n_1 + n_2$ observations and replace x_i by x and y_i by y.

Example: The ordered sample is $x_1, x_4, y_4, x_3, y_1, y_2, x_2, y_3$. Re-write the sample as $\underline{xx}\underline{y}\underline{x}\underline{yy}\underline{x}\underline{y}$. The total number of runs is 6, denoted by R.

If two distributions are the same, then the total number of runs will be high due to mixing. If two distributions are different, then the number of runs will be small. The number of ways to get combinations of $x's$ and $y's$ is,

$$P(R = 2k) = \frac{\binom{n_1 - 1}{k - 1}\binom{n_2 - 1}{k - 1}}{\binom{n_1 + n_2}{n_1}}$$

Suppose $k = 2$. Then, there are 4 possible runs: $xyxxyy$, $xyyxxy$, $xxyxyy$, $xxyyxy$. If R is odd:

$$P(R = 2k + 1) = \frac{\binom{n_1 - 1}{k}\binom{n_2 - 1}{k} + \binom{n_1 - 1}{k - 1}\binom{n_2 - 1}{k - 1}}{\binom{n_1 + n_2}{n_1}}$$

There can be $k+1$ runs of $x's$ and k runs of $y's$, or k runs of of $x's$ and $k+1$ runs of $y's$. Reject H_0 if $R \leq c$. For small n_1, n_2, we can find $p = P(R \leq r)$, r is the observed number of runs. For large n_1, n_2,

$$z\frac{R - \mu_R}{\sigma_R} \sim N(0, 1), \;\; \mu_R = \frac{2n_1n_2}{n_1 + n_2} + 1, \;\; \sigma_R^2 = \frac{(\mu_R - 1)(\mu_R - 2)}{(n_1 + n_2 - 1)}.$$

Reject H_0 if $z < -z_\alpha$.

7.19.10 Kolmogorov-Sminolv Goodness-of-fit Test

X has a cdf $F(x) = P(X \leq x)$. Test $H_0 : F(x) = F_0(x)$, where $F_0(x)$ is some given function. $x_1, x_2, ..., x_n$ is an iid sequence. The empirical distribution function is $F_n(x)\frac{n_x}{n}$, where n_x is the number of sample values less than or equal to x. Let $y_1, y_2, ..., y_n$ be an ordered sample.

$$F_n(x) = \begin{cases} 0, & \text{if } x < y_1. \\ \frac{k}{n}, & \text{if } y_k < y_{k+1}, k = 1, 2, n - 1. \\ 1, & \text{if } x \geq y_n. \end{cases}$$

$$W = F_n(x) = \frac{n_x}{n}, \;\; nW = n_x \sim Binomial(n, F(x)).$$

$$P(W = \frac{k}{n}) = P(nW = k) = \binom{n}{k} F(x)^k[1 - F9x)]^{n-k}, \;\; nE(W) = nF(x).$$

$E(W) = F(x)$. W is an unbiased estimator of $F(x)$. $F_n(x) \xrightarrow{p} F(x)$, as $n \to \infty$. The test statistic is $D_n = \sup_x |F_n(x) - F_0(x)| = \max(F_0(y_1), |F_n(y_i) - F_0(y_i)|, i = 1, 2, ..., n)$. The table on page 690 of the text book gives the distribution of D_n. Reject H_0 if $D_n \geq c$.

Example: Problem 10.7-1 on page 641 of the text book.

$$F_0(x) = \begin{cases} 0, & \text{if } x \leq 0. \\ x, & \text{if } 0 < x < 1 \\ 1, & \text{if } x \geq 1. \end{cases}$$

$d_{10} = |F_{10}(0.65) - F_0(0.65)| = |\frac{9}{10} - 0.65| = 0.25$. Note, order the sample, then look for $d_n = \max[f_0(y_1), |F_n(y_i) - F_0(y_i)|, i = 1, 2, ..., n]$. $\alpha = 00.1$, $d_{0.1}(10) = 0.37$. $P(D_{10} \geq d_1(10) = 0.1$. Thus, do not reject H_0.

Example: Use the distribution as before. $n = 5$ $0.4, 0.51, 0.53, 0.62, 0.74$.

i	y_i	$F_0(y_i)$	$F_n(y_i)$	$\lvert F_0 - F_n\rvert$
1	0.40	0.40	0.20	0.20
2	0.51	0.51	0.40	0.11
3	0.53	0.53	0.60	0.07
4	0.62	0.62	0.80	0.18
5	0.74	0.74	1	0.26

$d_5 = F_0(y_1) = 0.40$. $\alpha = 0.20$(given). $d_{0.2}(5) = 0.45$. Do not reject H_0.

7.20 Final Exam

Do eight problems.

1. Let $x_1, x_2, ..., x_n$ be a random sample from $N(\mu, \sigma^2)$. What is the MLE for μ^2? Find expected value of this estimator and use this to obtain an unbiased estimator of μ^2. Here σ is assumed to be unknown.

2. In order to estimate the percentage of a large class of college freshmen that had high school GPA's from 3.2 to 3.6 inclusive, a sample of $n = 50$ students was taken and only 9 of those fell in this class. Give a 95% confidence interval for the percentage of this freshmen class having a high school GPA of 3.2 to 3.6.

3. The pulse rate of a random sample of 15 workers from a mining town gives $\bar{x} = 82$ and $s^2 = 60$. Test if the mean pulse rate of the mining workers is 75. Use $\alpha = 0.01$ and state the assumptions that you need to make about the distribution of the pulse rate.

4. Commissioner Doc claims that 50% of the population of town A is indifferent to the construction of a new highway. In a random sample of 250 people, 110 are indifferent, 100 are in favor, and 40 are opposed to the new highway. Test at 5% level of significance if the Commissioner's claim is correct.

5. Over the past 10 years the following distribution of accidents was observed:

# accidents/mo	0	1	2	3	4	5	6	7	8	9	10 or more
# mos	2	10	15	30	28	12	10	6	2	1	1

   Are these data compatible with the hypothesis that the monthly accidents have a Poisson distribution with $\lambda = 4$?

6. Consider the following data on 1500 subjects and test the hypothesis that the severity of condition and blood type are independent.

	BLOOD TYPE			
Severity of Condition	A	B	AB	O
Absent	543	211	90	476
Mild	44	22	8	31
Severe	28	9	7	31

7. Consider the linear model $Y_i = \alpha + \beta(x_i - \bar{x}) + \epsilon_i, i = 1, 2, ..., n$. Derive $E(\hat{\alpha}), Var(\hat{\alpha})$ and $Var(\hat{\beta})$, where $\hat{\alpha} = \sum Y_i/n$ and $\hat{\beta} = \sum Y_i(x_i - \bar{x})/\sum(x_i - \bar{x})^2$. Giving an answer alone without proof is not sufficient. Here $E(\epsilon_i) = 0, Var(\epsilon_i = \sigma^2$, and x_i are fixed constants.

8. QPA of 10 students selected at random from ODU yielded: 2.5, 3.2, 3.5, 2.9, 3.7, 3.1, 2.8, 2.7, 3.4, 3.0. Carry out a test about the median for $H_0 : m = 2.8$ against $H_1 : m > 2.8$. Use an approximate 5% significance level.

9. Let $X_1, ..., X_n$ and $Y_1, ..., Y_m$ be two random samples. Let $R_i, i = 1, 2, ..., m$, be the rank of Y_i in a combined sample of $n + m$ observations. If $T = \sum_i^{R_i}$, then find $E(T)$ for test $H_0 : m_x = m_y$ against $m_x > m_y$ would you reject H_0 for "large" observed values of T or "small" observed values of T?

10. (a) Write down H_0 and H_1 for the Run Test.

    (b) In two samples of size $n_1 = n_2 = 5$, let the observed values of R be $r = 4$. Find p-value for the Run Test.

7.21 Homework

10.1-3:

$$f(x) = \frac{e^{-\frac{x}{3}}}{3}, \quad F(y) = \int_0^y \frac{e^{-\frac{x}{3}}}{3}\,dx = 1 - e^{-\frac{y}{3}} = P(X_i \le y).$$

(a)

$$g_r(y) = \sum_{k=3}^{4} \left(\begin{array}{c} 5 \\ k \end{array} \right) (k)F(y)^{k-1} f(y)[1 - F(y)]^{5-k} = 10[1 - e^{-\frac{y}{3}}]e^{-y}, 0 \le y \le \infty.$$

$$P(Y_4 < 5) = \left(\begin{array}{c} 5 \\ 4 \end{array} \right) [1 - e^{-\frac{y}{3}}]^4 e^{-\frac{y}{3}}.$$

(b)

$$[1 - e^{-\frac{y}{3}}]^5 = 0.76.$$

(c)

$$P(1 < Y_1) = \sum_{k=0}^{0} \left(\begin{array}{c} 5 \\ k \end{array} \right) [1 - e^{-\frac{y}{3}}]^k [e^{-\frac{y}{3}}]^{5-k} = 0.188876.$$

10.1-7 $n = 72, \prod_{\frac{1}{3}} = 7.2$.

(a)

$$P(Y_{20} < \prod_{\frac{1}{3}} = 7.2) = \sum_{k=20}^{72} \left(\begin{array}{c} 72 \\ k \end{array} \right) \left(\frac{1}{3}\right)^k \left(\frac{2}{3}\right)^{72-k}.$$

Estimating using the Poisson distribution, $\lambda = 72\left(\frac{1}{3}\right) = 26; x = 20$. $P(Y_{20} < 7.2) = 1 - 0.13867 = 0.86133$. Using the Normal distribution,

$$P(Y_{20} < 7.2) = 1 - \Phi\left(\frac{19.5 - 24}{\sqrt{16}}\right) = 1 - \Phi(-1.125) = 0.87.$$

(b)

$$P(Y_{18} < \prod_{\frac{1}{3}} < Y_{30}) = \sum_{k=18}^{29} \left(\begin{array}{c} 72 \\ k \end{array} \right) \left(\frac{1}{3}\right)^k \left(\frac{2}{3}\right)^{72-k} = \Phi\left(\frac{29.5 - 24}{4}\right) - \Phi\left(\frac{17.5 - 24}{4}\right) =$$

$$\Phi(1.35) - \Phi(-1.625) = 0.915 - 0.05169 = 0.8634.$$

10.1-10 $X \sim U(0, \theta)$.

(a)

$$f(x) = \frac{1}{\theta}, \prod_{i=1}^{n} \frac{1}{\theta} = \frac{1}{\theta^n} = L(\theta), \ \log L(\theta) = -n \log \theta, \ \frac{\partial \log L}{\partial \theta} = -\frac{n}{\theta} = 0.$$

Can't solve for a non-trivial θ. So, look at the graph in Figure 7.1.

(b) Note that

$$F(y) = \int \frac{1}{\theta}\, dy = \frac{y}{\theta}.$$

Then,

$$g_n(y) = n\left(\frac{y}{\theta}\right)^{n-1} \frac{1}{\theta} = \frac{ny^{n-1}}{\theta^n}, \ \ E(Y_n) = \int_0^\theta y g_n(y)\, dy = \int_0^\theta \frac{ny^n}{\theta^n}\, dy = \frac{n\theta}{n+1}.$$

Use that to find the variance.

$$E(Y_n^2) = \int_0^\theta y^2 g_n\, dy = \int_0^\theta y^2 \frac{ny^{n-1}}{\theta^n} = \frac{n\theta^{n+2}}{(n+2)\theta^n} = \frac{n\theta^2}{n+2}.$$

$$Var(Y_n) = E[(Y_n - \mu)^2] = E[Y_n^2] - [E[Y_n]^2 = \frac{n\theta^2}{n+2} - \frac{n^2\theta^2}{(n+1)^2} = \ldots = \frac{\theta^2 n}{(n+2)(n+1)^2}.$$

(c) $\frac{nY_n}{n+1}$ is a biased estimator of θ. Set $c = \frac{n+1}{n}$ to make it an unbiased estimator.

10.2-1 **(a)**

$$P(Y_2 < \prod_{0.5} < Y_5) = \sum_{k=2}^{4} \left(\begin{array}{c} 6 \\ k \end{array} \right) \left(\frac{1}{2}\right)^k \left(\frac{1}{2}\right)^{6-k} = 0.2344 + 0.3125 + 0.234375 = 0.78125.$$

(b)

$$P(Y_1 < \prod_{\frac{1}{4}} < Y_4) = \sum_{k=1}^{3} \left(\begin{array}{c} 6 \\ k \end{array} \right) \left(\frac{1}{4}\right)^k \left(\frac{3}{4}\right)^{6-k} = 0.35596 + 0.296631 + 0.131836 = 0.7844.$$

(c)

$$P(Y_4 < \prod_{0.9} < Y_6) = \sum_{k=4}^{5} \left(\begin{array}{c} 6 \\ k \end{array} \right) \left(\frac{9}{10}\right)^k \left(\frac{1}{10}\right)^{6-k} = 0.098415 + 0.354294 = 0.4527.$$

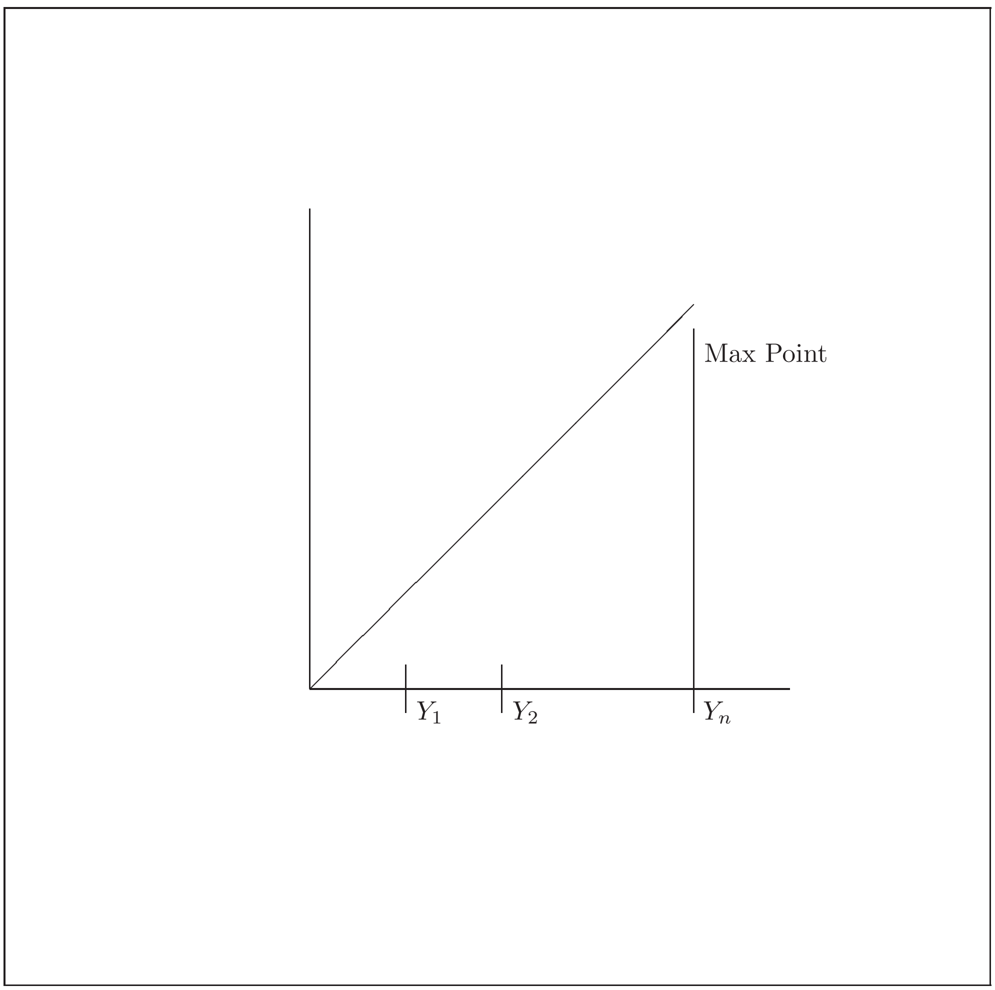

Figure 7.1:

10.2-3 **(a)** $P(Y_i < \prod_{\frac{1}{2}} < Y_j) = 0.05$. Find i, j.

$$\frac{i - 0.5 - 10(\frac{1}{2})}{\sqrt{10(0.5)(0.5)}} = -z_{\alpha/2} = -1.96 \Rightarrow i = 2.4$$

$$\frac{j - 0.5 - 10(\frac{1}{2})}{\sqrt{10(0.5)(0.5)}} = z_{\alpha/2} = 1.96 \Rightarrow j = 8.599.$$

Thus, $(Y_2 = 110, Y_9 = 137)$.

(b) $P(Y_2 < \prod_{\frac{1}{2}} < Y_9) = (0.9786)100 = 97.86\%$ by Table 10.2-1 on page 602.

10.3-3 $\alpha = 0.0662, \alpha/2 = 0.0331, n = 24$, $\hat{m} = \frac{1}{2}Y_{12} + \frac{1}{2}Y_{13} = 4$. $W = \#x_i - y_i > 0 = 13 = \# + signs$. Using Table II, $c_1 = 7, c_2 = 17$. Since $13 \geq 7$ and $13 \leq 17$, do not reject the null hypothesis. $H_0 : m_0 = 0$. $H_1 : m_0 \neq 0$.

10.3-8

Student	Difference
1	-3
2	1
3	4
4	-3
5	-3
6	4
7	-3
8	5
9	6
10	6
11	-2
12	4
13	6
14	4
15	4

$H_0 : m_D = 0$. $H_1 : n_D \neq 0$. $\alpha = 0.1, n = 15$. $W = \#+$ signs $= 10$. Using Table II, $c_1 = 4, c_2 = 10$. Since $W \geq 10$, reject the null hypothesis.

10.4-7 $n = 15$. $H_0 : m = 0$. $H_1 : m > 0$.

$x-y$	Rank $\|x-y\|$
-0.34	15
0.18	8
0.22	12
0.17	7
-0.07	3
0.22	12
0.19	9
0.06	2
0.22	12
0.04	1
-0.13	5
0.23	14
0.16	6
-0.21	10
0.09	4

$W = -15 + 8 + 12 + 7 - 3 + 12 + 9 + 2 + 12 + 1 - 5 + 14 + 6 - 10 + 4 = 54$. $z_{0.05} = 1.645$. $z = \frac{W}{\sqrt{\frac{(15)(16)31}{6}}} = \frac{54}{35.213} = 1.533$. Since $1.533 < 1.645$, fail to reject the null hypothesis.

10.5-2 (a)

Data	Rank
0.7494	1
0.7546	2
0.7565	3
0.7613	4(y)
0.7615	5
0.7701	6
0.7712	7
0.7719	8.5
0.7719	8.5
0.7720	10.5
0.7720	10.5(y)
0.7731	12(y)
0.7741	13
0.7750	14.5
0.7750	14.5(y)
0.7776	16
0.7795	17(y)
0.7811	18(y)
0.7815	19(y)
0.7816	20(y)
0.7851	21(y)
0.7870	22(y)
0.7876	23(y)
0.7972	24(y)

$W = 4 + 10.5 + 12 + 14.5 + 17 + 18 + 19 + 20 + 21 + 22 + 23 + 24 = 205$. $z = \frac{205 - \frac{12(25)}{2}}{\sqrt{\frac{(12)(12)(25)}{12}}} = 3.175$. Since $3.175 > 1.645$, reject the null hypothesis.

$$p = P(W \geq 205) = P\left(\frac{W - 150}{\sqrt{300}} \geq \frac{205 - 150}{\sqrt{300}}\right) = P(Z \geq 3.175) = 0.0008.$$

(b) $V = 9$.

$$P(V=v) = \frac{\binom{12}{v}\binom{12}{12-v}}{\binom{24}{12}} = h(v).$$

$$h(9) = \frac{\binom{12}{9}\binom{12}{3}}{\binom{24}{12}} = 0.0178984, \quad h(10) = \frac{\binom{12}{10}\binom{12}{2}}{\binom{24}{12}} = 0.001611,$$

$$h(11) = \frac{\binom{12}{11}\binom{12}{1}}{\binom{24}{12}} = 0.000053251, \quad h(12) = \frac{\binom{12}{12}\binom{12}{0}}{\binom{24}{12}} = 0.000000369.$$

$p = P(V \geq 9) = h(9) + h(10) + h(11) + h(12) = 0.0196$. Since $9 \geq 9$, reject the null hypothesis.

10.6-1 $n_1 = n_2 = 8$. The ordered set is $4.95, 5, 5.2, 5.4, 5.45, 5.5, 5.55, 5.7, 5.75, 5.85, 6, 6.05, 6.2, 6.25, 6.55, 6.65$. The run set is: $\underline{xxxxx}\overline{y}\underline{xx}\overline{yyx}\underline{yyyyy}$. Total runs is $r = 6$.

$$P(R=2) = \frac{2\binom{7}{0}\binom{7}{0}}{\binom{16}{8}} = \frac{2}{12870}, \quad P(R=3) = \frac{\binom{7}{1}\binom{7}{0} + \binom{7}{0}\binom{7}{1}}{12870} = \frac{14}{12870}.$$

$$P(R=4) = \frac{2\binom{7}{1}\binom{7}{1}}{12870} = \frac{28}{12870}, \quad P(R=5) = \frac{\binom{7}{2}\binom{7}{1} + \binom{7}{1}\binom{7}{2}}{12870} = \frac{294}{12870}.$$

$$P(R=6) = \frac{2\binom{7}{2}\binom{7}{2}}{12870} = \frac{882}{12870}.$$

$\alpha = 0.10$. $c : (r : r \leq 6)$, $\hat{\alpha} = \frac{1220}{12870} = 0.095$. Since $6 = 6$, reject H_0.

10.7-8

$$F_0(x) = \sum_{x=0}^{x} \frac{5.6^x e^{-5.6}}{x!} = P(X \leq x).$$

i	Y_i	$F_0(Y_i)$	$F_n(Y_i)$	$\lvert F_0 - F_n \rvert$
1	0	0.0037	0	0.0037
2	1	0.0244	0	0.0244
3	2	0.0824	$\frac{2}{62}$	0.0501
4	3	0.1906	$\frac{10}{62}$	0.0293
5	4	0.3421	$\frac{17}{62}$	0.0679
6	5	0.5118	$\frac{30}{62}$	0.0279
7	6	0.6702	$\frac{43}{62}$	0.0233
8	7	0.7970	$\frac{53}{62}$	0.0578
9	8	0.8857	$\frac{57}{62}$	0.0337
10	9	0.9408	$\frac{61}{62}$	0.0431
11	10	0.9718	1	0.0282

$\max(0.0037, 0.0679) = 0.0679$. $d_{62} = 0.0679; d_{0.1} = 0.1549$. Since $0.0679 < 0.1549$, do not reject the null hypothesis.

Chapter 8

Design and Analysis of Experiments

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STAT 535, Spring 1996

Text used: Petersen, Roger G. *Design and Analysis of Experiments,* Marcel Dekker, Inc, New York, New York 1985

8.1 Terminology

1. An *experiment* is a planned inquiry to discover new facts or to confirm or deny the results of the previous investigations.

2. A *treatment* is a procedure whose effect on the experimental material is to be measured. For example, two varieties of wheat form two treatments.

3. A particular class of related treatments is called a *factor.* For example, variety of wheat is a factor. Quenching solution is a factor.

4. The states of a factor, that is, the treatments within the class are called the *levels* of the factor.

   Example: In an agricultural experiment, two varieties of wheat are being compared along three levels of a fertilizer brand. Here, wheat variety is a factor, into two levels and fertilizer brand is another factor with three levels. A treatment in this experiment would be a combination of one level of variety of wheat with one level of fertilizer. Thus, there are $2(3) = 6$ treatments.

5. An *experimental unit* is the piece of experimental material to which one trial of a single treatment is applied.

6. A *sampling unit* is that fraction of the experimental unit on which the effect of the treatment is measured. In the agricultural experiment, plots in a piece of land are the experimental units. Take two square yards in a plot. That would be a sample unit.

7. A group of homogeneous experimental units is called a *block.*

8. The quantity that is measured on the experimental material is often called the *yield.*

9. An *experimental design* is a set of rules by which treatments to be used in an experiment are assigned to the experimental units.

10. *Experimental error* is the variation among experimental units which have been treated alike.

11. If treatments are assigned to a set of units in such a way that every unit is equalikely to receive any treatment, then the assignment is said to be *random.*

12. When a treatment appears more than once in an experiment, the treatment is said to be *replicated.*

13. The *experimental unit* is the physical entity or subject exposed to the treatment independently. The experimental unit, upon exposure to the treatment, constitutes a single replication.

14. *Experimental error* describes the variation of many identically treated experimental units.

15. The *sampling(observational) unit* is a sample from the experimental unit(e.g. individual plants sampled from a field or serum samples from a subject).

16. *Sampling error* is the variation among sampling units.

Almost all experimentation is done for one or both of these purposes:

1. Testing of hypotheses about the effects of the different treatments.

2. Estimating the differences among different treatments.

An additional purpose is to obtain information on why treatment affects the experimental material as they do. The role of experimental design is to provide efficient and precise information to meet these objectives. In addition, conducting experiments are to provide assessments of estimates and to estimate variability of the experimental material. A good experimental design should have at least three features:

1. Replication. Replication is needed to estimate variations in the experimental units.

2. Randomization. Replication is not the only factor that must be considered in designing the experiment. A good experimental design should assign the treatments to the experimental units randomly.

3. Blocking. A good experimental design should have blocking for the purpose of controlling sources of variability among experimental units.

Analysis of the data obtained is done using *analysis of variance* techniques. This is a systematic procedure for partitioning the total variation among the observations into components each of which is associated with a source of variation.

8.2 Completely Randomized Design(CRD)

Example: Two types of animal diet, diet A and diet B. See Figure 8.1.
Animals in pen A are assigned diet A. Animals in pen B are assigned diet B. The experimental units are the two pens. The treatments are diet A and diet B. No replications are performed. There are six sampling units in each pen. There is no data to estimate experimental error. But, the sampling error can be estimated.

Example: The previous example can be modified to have replications. See figure 8.2.

Randomly assign diet A and diet B to the pens. This way, we have two replications of each. The variance of the random error can be estimated.

The simplest and the least restrictive design is the Completely Randomized Design. In general, there are p treatments and n experimental units. $n > p$. Randomly select r_1 experimental units from n and assign treatment 1. Next, randomly select r_2 experimental units from $n - r_1$ units and assign treatment 2. Continue the procedure until the n experimental units have been used. This design utilizes randomization and replication. If $r_1 = r_2 = \cdots = r_p$, then the results are more efficient.

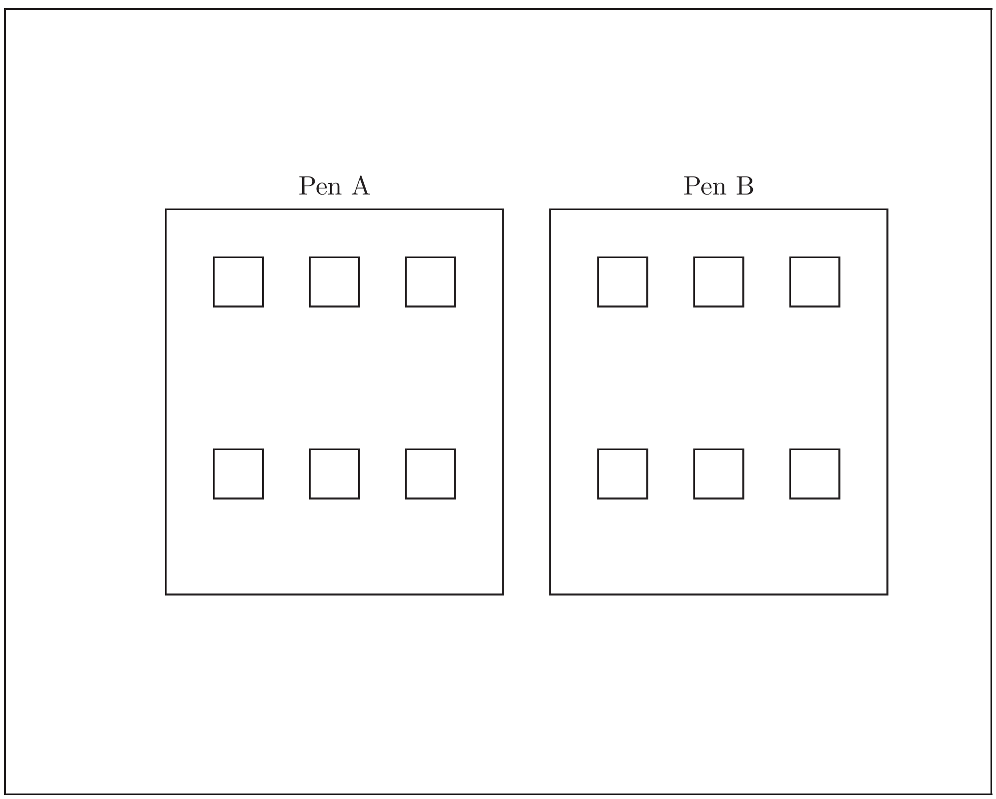

Figure 8.1:

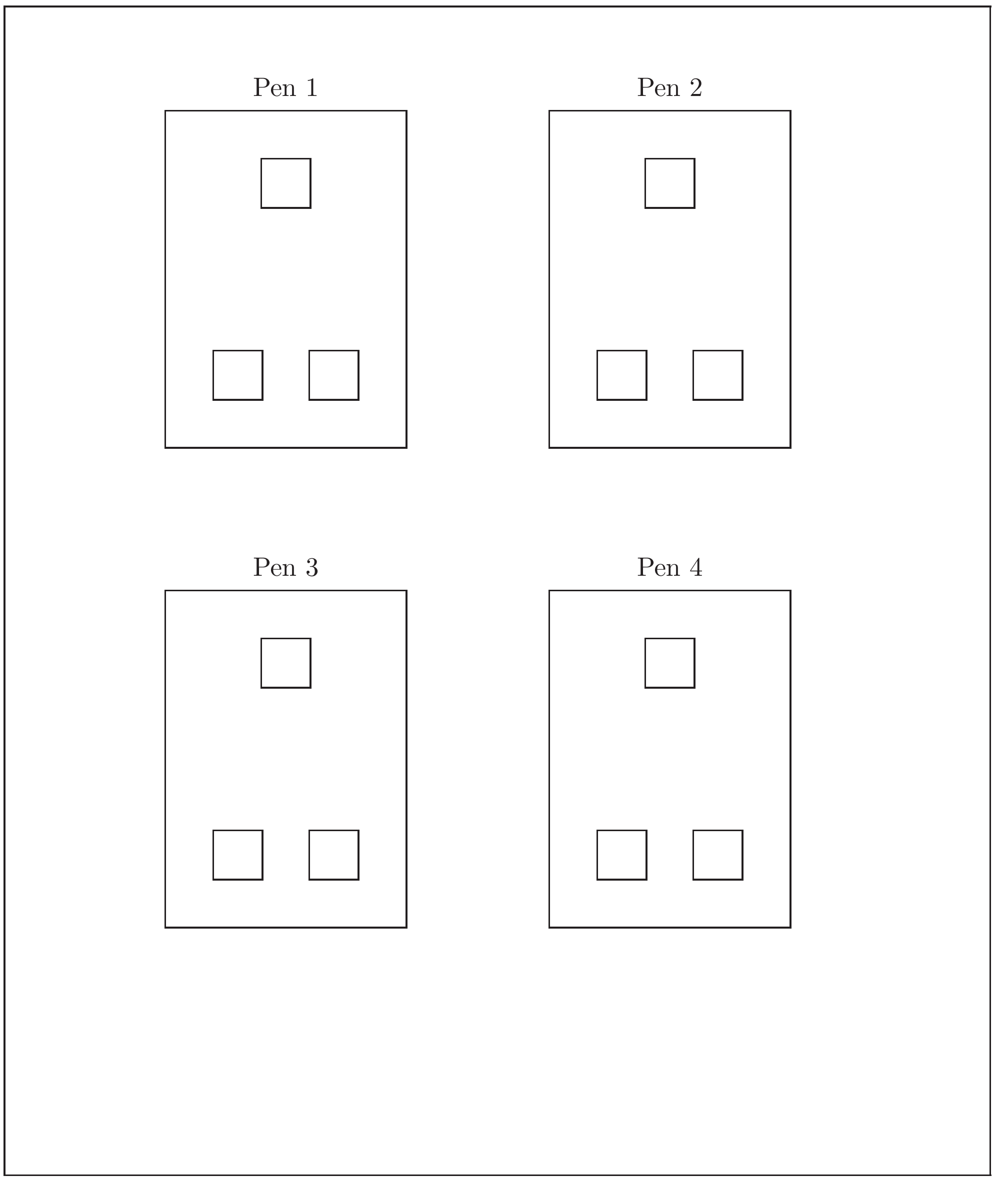

Figure 8.2:

Example: Suppression of bacterial growth in stored meats. Recent studies suggested controlled gas atmospheres as possible alternatives to existing packing methods. The packaging methods are as follow:

- Wrap.
- Vacuum.
- 1% CO_2, 40% O_2, 5% N.
- 100% CO_2.

A CRD design was used. There were three beef steaks of approximately the same size (75g) for each treatment. We randomly assigned to each steak the four packaging conditions. Thus, there are a total of 12 beef steaks. Measurements of the growth of pserotrozic bacteria on the meat 9 days after packing were made. The data is presented in the following table:

Packing Condition	$\log(count/cm^2)$
Wrap	7.66, 6.98, 7.8
Vacuum	5.26, 5.44, 5.8
1% CO_2, 40% O_2, 5% N	7.41, 7.33, 7.04
100% CO_2	3.51, 2.91, 3.66

In general, data obtained using CRD looks like this:

Treatments			
1	2	...	p
y_{11}	y_{21}	$\cdots$	y_{p1}
y_{12}	y_{22}	$\cdots$	y_{p2}
.	.	.	.
.	.	.	.
.	.	.	.
y_{1r}	y_{2r}	$\cdots$	y_{pr}

Note that all the measurements must be independent. The following problems are of importance:

1. Estimate the true mean yields for p treatments.
2. Test the significance of the differences among the treatment means.
3. Obtain an estimate of the standard deviation of treatment means, so that the confidence interval for the treatment mean can be constructed.

We need a model to answer these questions. A linear means model is used. The *means model* is $y_{ij} = \mu_i + \epsilon_{ij}, i = 1, 2, ..., p; j = 1, 2, ..., r$. μ_i is the mean of the i-th population. Assume that there are p populations with means $\mu_1, \mu_2, ..., \mu_p$ and with a common variance, σ^2. In the model, ϵ_{ij} is the experimental error, $E(\epsilon_{ij}) = 0$ and $Var(\epsilon_{ij}) = \sigma^2$.

$$E(y_{ij}) = E(\mu_i + \epsilon_{ij}) = \mu_i + E(\epsilon_{ij}) = \mu_i + 0.$$

$$Var(y_{ij}) = Var(\mu_i + \epsilon_{ij}) = Var(\epsilon_{ij}) = \sigma^2.$$

The hypothesis test concerning the treatment means is stated as, $H_0 : \mu_1 = \mu_2 = \cdots = \mu_p$.

8.2.1 Estimation of Model Parameters

The parameters of the means model are $\mu_1, \mu_2, ..., \mu_p$ and σ^2. The method of least squares is used on linear models to estimate the means. The method minimizes the sum of squares of the errors.

$$\sum_{i=1}^{p}\sum_{j=1}^{r}\epsilon_{ij}^2 = \sum_{i=1}^{p}\sum_{j=1}^{r}(y_{ij}-\mu_i)^2$$

is a minimum. The estimators used are:

$$\hat{\mu}_1 = \bar{y}_{1\cdot} = \frac{1}{r}\sum_{j=1}^{r} y_{ij},\ \hat{\mu}_2 = \bar{y}_{2\cdot} = \frac{1}{r}\sum_{j=1}^{r} y_{ij},\ ...,\ \hat{\mu}_p = \bar{y}_{p\cdot} = \frac{1}{r}\sum_{j=1}^{r} y_{ij},$$

The estimator of the experimental error is $\hat{\epsilon}_{ij} = y_{ij} - \hat{\mu}_i$. Let ξ be a random variable. $E(\xi) = 0$ and $Var(\xi) = \sigma^2$. Then, we have $\hat{\xi}_{11}, \hat{\xi}_{21}, ..., \hat{\xi}_{p1}$. A pooled variance formula is given by,

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^{p}\sum_{j=1}^{r}(y_{ij}-\bar{y}_{i\cdot})^2}{r(p-1)}.$$

8.2.2 Standard errors of $\hat{\mu}_i$

Consider the parameters $\mu_1, \mu_2, ..., \mu_p$. We have obtained $\hat{\mu}_1 = \bar{y}_1, ..., \hat{\mu}_p = \bar{y}_p$. Find the standard deviation of $\hat{\mu}_i = \bar{y}_{i\cdot}, i = 1, 2, ..., p$. $Var(\bar{y}_{i\cdot}) = \frac{\sigma^2}{r}, i = 1, 2, ..., p$. The standard deviation is $\frac{\sigma}{\sqrt{r}}, i = 1, 2, ..., p$. The standard error of $\bar{y}_{i\cdot}$ is simply the estimated standard deviation of $\bar{y}_{i\cdot}$. The standard error of $\bar{y}_{i\cdot} = \frac{\hat{\sigma}}{\sqrt{r}}$. Thus, for $\mu_i = \bar{y}_i$ and the standard error of $\hat{\mu}_i = \frac{\hat{\sigma}}{\sqrt{r}}$.

8.2.3 Confidence Interval for μ_i

$\hat{\mu}_i = \bar{y}_{i\cdot}$. The standard error is given by $\frac{s}{\sqrt{r}}$. A 100% confidence interval is $\hat{\theta} \pm z_{\alpha/2}SE(\hat{\theta})$. So, an approximate confidence interval is given by, $\bar{y}_{i\cdot} \pm z_{\alpha/2}\frac{s}{\sqrt{r}}$. To get an exact confidence interval, use the assumption of Normal distribution for the population. Then, $\hat{\mu}_i = \bar{y}_{i\cdot} \sim N\left(\mu_i, \frac{\sigma^2}{r}\right)$. Further more,

$$p(r-1)\hat{\sigma}^2 = \sum_i\sum_j(y_{ij}-\bar{y}_{i\cdot})^2 \sim \chi^2(p(r-1))$$

and is an exact value of $y_{i\cdot}$. Then,

$$\frac{\bar{y}_{i\cdot} - \mu_i}{\frac{s}{\sqrt{r}}} \sim t(p(r-1)).$$

Then, a $100(1-\alpha)\%$ exact confidence interval for μ_i is:

$$y_{i\cdot} \pm t_\alpha(p(r-1))\frac{s}{\sqrt{r}}.$$

8.2.4 Testing of Hypotheses

One important hypothesis of interest is to test the equality of all treatment means. That is, test H_0 : $\mu_1 = \mu_2 = \cdots = \mu_p$ versus $H_a : \mu_i \neq \mu_j$, for at least one $(i, j), i \neq j$. For testing H_0, consider the following decomposition of the total sum of squares.

$$\sum_{i=1}^{p}\sum_{j=1}^{r}(y_{ij}-\bar{y})^2 = \sum_{i=1}^{p}\sum_{j=1}^{r}(y_{ij}-\bar{y}_{i\cdot})^2 + r\sum_{i=1}^{p}(y_{i\cdot}-\bar{y})^2.$$

The above equation is called the *sum of squares* or *sum of squares due to error.* $SS(E) + SS(TRT)$. Note that

$$\bar{y} = \frac{1}{rp}\sum_{i=1}^{p}\sum_{j=1}^{r} y_{ij} = \frac{1}{p}\sum_{i=1}^{p}\bar{y}_{i\cdot}.$$

Intuitively, it is clear that if H_0 is true, then $SS(TRT)$ will be small and a small value of this, $\frac{\frac{SS(TRT)}{p-1}}{\frac{SS(E)}{p(r-1)}}$ would support the null hypothesis. More formally, we can show the following when the Normal distribution assumption is made:

1. $SS(E) = \sum_{i=1}^{p}\sum_{j=1}^{r}(y_{ij} - \bar{y}_{i\cdot})^2 \sim \chi^2(p(r-1))$.
2. $SS(TRT) = r\sum_{i=1}^{p}(\bar{y}_{i\cdot} - \bar{y})^2 \sim \chi^2(p-1)$ under the null hypothesis.
3. The true sum of squares in (1) and (2) are independent. Let $x \sim \chi^2_{v_1}$ and $y \sim \chi^2_{v_2}$ be independent. Then, $F = \frac{\frac{x}{v_1}}{\frac{y}{v_2}}$.
4. Under $H_0 : F = \frac{\frac{SS(TRT)}{p-1}}{\frac{SS(E)}{p(r-1)}}$. Thus, to test H_0 we reject H_0 if $F > F_\alpha(p-1, pr-1)$, where it is useful to note that
   (a) $E\left[\frac{SS(E)}{p(r-1)}\right] = \sigma^2$.
   (b) $E\left[\frac{SS(TRT)}{p-1}\right] = \sigma^2 + \frac{1}{p-1}\sum_{i=1}^{p}(\mu_{i\cdot} - \bar{\mu})^2$, $\bar{\mu} = \frac{1}{p}\sum_{i=1}^{p} p_i$.
   (c) (a) and (b) are independent.

All of the above results are summarized in a table called an *ANOVA Table.*

Source	d.f.	SS	MS	F
Treatment	p-1	SS(TRT)	$\frac{SS(TRT)}{p-1}$	$\frac{MS(TRT)}{MS(E)}$
Error	$p(r-1)$	SS(E)	$\frac{SS(E)}{p(r-1)}$	
Total	$pr-1$	SS(TOT)		

$$SS(TRT) = r\sum_{i=1}^{p}(y_{i\cdot} - \bar{y})^2,\ SS(E) = \sum_{i=1}^{p}\sum_{j=1}^{r}(y_{ij} - \bar{y}_{i\cdot})^2,\ SS(TOT) = \sum_{i=1}^{p}\sum_{j=1}^{r}(y_{ij} - \bar{y})^2.$$

Recall the storage of meat example. $p = 4, r = 3$. Test $H_0 : \mu_1 = \mu_2 = \mu_3 = \mu_4$. Using SAS software, we can do the analysis. (1) Create a data set with two variables,

```
DATA A;
INPUT TRT Y;
CARDS;
COMMON Y11 Y12 Y13
VACU Y21 Y22 Y23
COO2N Y31 Y32 Y33
CO2 Y41 Y42 Y43
;
```

and (2) use the PROC ANOVA method in SAS:

```
PROC ANOVA;
CLASS TRT;
MODEL Y=TRT;
RUN;
```

8.2.5 Data Obtained Using CRD

To analyze the data, consider the model, $y_{ij} = \mu_i + \epsilon_{ij}, i = 1, 2, ..., p; j = 1, 2, ..., r$. y_{ij} is the j-th observation on the i-th treatment. μ_i is the mean due to the i-th treatment. ϵ_{ij} is random error. The assumptions of the linear one-way model are:

1. ϵ_{ij} is an iid sequence with a Normal distribution.
2. $E(\epsilon) = 0$.
3. $Var(\epsilon) = \sigma^2$.

For the meat packing problem, the ANOVA table looks like this:

Source	d.f.	SS	MS	F	p-value
Treatment	3	32.8728	10.9576	94.58	0.0001
Error	8	0.9268	0.11585		
Total	11	33.7996			

The F statistic and p-value are used to test, $H_0 : \mu_1 = \mu_2 = \mu_3 = \mu_4$. $H_a : \mu_i \neq \mu_j, i \neq j \in 1...4$. The p-value is $P(F(3, 8) > 94.58)$. For small p-values, we reject the null hypothesis. In this case, the null hypothesis is rejected. Next, estimate μ_i and σ^2. From the ANOVA table, $\hat{\sigma}^2 = 0.11585$. To get the treatment means using SAS, use the following source code:

```
PROC SORT;
BY TRT;

PROC MEANS;
BY TRT;
VAR YI;
RUN;
```

The means produced are $\hat{\mu}_1 = 7.48, \hat{\mu}_2 = 5.5, \hat{\mu}_3 = 7.26, \hat{\mu}_4 = 3.36$. The standard error of $\hat{\mu}_i = \frac{s}{\sqrt{r}} = \frac{\sqrt{0.1155}}{\sqrt{3}} = 0.197$. A 95% confidence interval for μ_4 would be: $\hat{\mu}_4 \pm t_{0.025}(pr-1)(0.197) = 3.36 \pm 2.306(0.197) = 3.36 \pm 0.454$.

8.2.6 Another Form of 1-Way ANOVA Model

This is also known as a treatment effects model. The model statement is $y_{ij} = \mu + \tau_i + \epsilon_{ij}$. μ represents the overall mean, τ_i is the effect of the i-th treatment, and ϵ_{ij} is still random error.

Example: p-drugs for treating headaches. n experimental units. μ would be the time headache goes away without drugs(the control value).

An assumption that goes with this model is $\sum_{i=1}^{p} \tau_i = 0$.

8.2.7 Unequal Replications

Unequal replications may occur for some experimental units that were lost during the study; there were an insufficient number of subjects for the study; collected data was lost, or destroyed or invalid. The notation for the degrees of freedom and sum of squares changes in the ANOVA table. However, the rest of the ANOVA table remains the same.

Source	d.f.	SS	...
Treatment	$p-1$	$\sum_{i=1}^{p} r_i(\bar{y}_{i\cdot} - \bar{y})^2$	...
Error	$\sum_{i=1}^{p} r_i - p$	$\sum_{i=1}^{p}\sum_{j=1}^{r_i}(y_{ij} - \bar{y}_{i\cdot})^2$	...
Total	$\sum_{i=1}^{p} r_i - 1$		

To estimate μ_i :

$$\hat{\mu}_i = \bar{y}_{i\cdot} = \frac{1}{r_i}\sum_{j=1}^{r_i} y_{ij}, \quad SE(\hat{\mu}_i) = \frac{s}{\sqrt{r_i}}, i = 1, 2, ..., p.$$

8.3 Contrasts

Recall the meat packing example. We rejected the null hypothesis because the p-value was very small. Some of the means are significantly different. We may be interested in some of these questions:

1. Is pure CO_2 more effective than the mixture of gases? $H_0 : \mu_3 = \mu_4$.
2. Are the gases more effective in reducing bacteria growth than a complete vacuum? $H_0 : \frac{1}{2}(\mu_3 + \mu_4) - \mu_2 = 0$.

A *contrast* of p means, say $\mu_1, \mu_2, ..., \mu_p$, is a linear combination $k_1\mu_1 + k_2\mu_2 + \cdots + k_p\mu_p$, with $\sum_{i=1}^{p} k_i = 0$. In our example, $\mu_3 - \mu_4 = (0)\mu_1 + (0)\mu_2 + (1)\mu_3 + (-1)\mu_4$ is a contrast. $k_1 = 0, k_2 = 0, k_3 = 1, k_4 = -1$. $\sum_{i=1}^{4} k_i = 0$. Similarly, $\frac{1}{2}(\mu_3 + \mu_4) - \mu_2$ is a contrast. $k_1 = 0, k_2 = -1, k_3 = \frac{1}{2}, k_4 = \frac{1}{2}$.

8.3.1 Estimation of Contrasts

Let $\theta = \sum_{i=1}^{p} k_i\mu_i, \sum_{i=1}^{p} k_i = 0$ be a contrast. Estimate θ. $\hat{\theta} = \sum_{i=1}^{p} k_i\hat{\mu}_i = \sum_{i=1}^{p} k_i\bar{y}_{i\cdot}$. The standard error of $\hat{\theta}$ is given by,

$$Var(\hat{\theta}) = Var\left(\sum_{i=1}^{p} k_i\bar{y}_{i\cdot}\right) = \sum_{i=1}^{p} k_i^2 Var(\bar{y}_{i\cdot}).$$

The treatment means are uncorrelated. $Var(\hat{\theta}) = \sigma^2\sum_{i=1}^{p}\frac{k_i^2}{r_i}$ for the unequally replicated case. For the equally replicated case,

$$Var(\hat{\theta}) = \frac{\sigma^2}{r}\left(\sum_{i=1}^{p} k_i^2\right).$$

Therefore, the standard error of $\hat{\theta}$ is

$$s\sqrt{\sum_{i=1}^{p}\frac{k_i^2}{r_i}} = \frac{s}{\sqrt{r}}\sqrt{\sum_{i=1}^{p} k_i^2},$$

if there is equal replication. To test $H_0 : \theta = 0$(the contrast is not significant), the test statistic F is given by

$$\frac{\left[\sum_{i=1}^{p} k_i\bar{y}_i\right]^2}{s^2\sum_{i=1}^{p}\frac{k_i^2}{r_i}} \sim F\left(1, \sum_{i=1}^{p} r_i - p\right).$$

or $F = \frac{SS(CONTRAST)}{MSE}$. The sum of squares of the contrast is given by,

$$\frac{\left(\sum_{i=1}^{p} k_i\bar{y}_{i\cdot}\right)^2}{\sum_{i=1}^{p}\frac{k_i^2}{r_i}}.$$

We have $\hat{\theta}, \theta : SE(\hat{\theta})$

$$t = \frac{\hat{\theta}}{SE(\hat{\theta})} \sim t\left(\sum_{i=1}^{p} r_i - p\right), \quad t^2 \sim F\left(1, \sum_{i=1}^{p} r_i - p\right).$$

To use SAS to test for the significance of contrast, implement the following source code:

```
DATA STEAK;
INPUT TRT Y;
...

PROC GLM;
CLASS TRT;
MODEL Y=TRT;
CONTRAST ‘C1’ TRT 0 0 1 -1;
CONTRAST ‘C2’ TRT 0 2 -1 -1;
```

The contrast table would look like this:

Contrast	d.f.	Contrast SS	Mean SS	F	p-value
C1	1	4.6464	4.6464	40.11	0.0002
C2	1	2.42	2.42	20.89	0.0018

Test $\theta_1 = \mu_3 - \mu_4 = 0$. $F = \frac{SS(CONTRAST)}{MS(E)} = \frac{4.6464}{0.1155}$. Compare the F value with $F(1, 8)$ for the θ_1 test. The p-value says to reject $H_0 : \theta_1 = 0$, $H_a : \theta_1 \neq 0$. To find the estimate and the standard error of the estimate of a contrast of means, use the following SAS code:

```
PROC ANOVA;
CLASS TRT;
MODEL Y=TRT;
ESTIMATE ‘C1’ TRT 0 0 1 -1;
ESTIMATE ‘C2’ TRT 0 2 -1 -1;
```

The code gives the estimated standard error and a t-test for H_0.

For the comparison of means, let $y_1 \sim N(\mu_1, \sigma^2)$, and $y_2 \sim N(\mu_2, \sigma^2)$ and y_1, y_2 are iid. The means are $\bar{y}_1$ and $\bar{y}_2$. The pooled standard deviation is

$$s = \sqrt{\frac{\sum_{i=1}^{p}(y_{1i} - \bar{y}_1)^2 + \sum_{i=1}^{p}(y_{2i} - \bar{y}_2)^2}{2n - 2}}.$$

Test $H_0 : \mu_1 - \mu_2 = 0$, $H_a : \mu_1 - \mu_2 \neq 0$. The two sample t-test rejects H_0 if $|t| \geq t_{\alpha/2}(2(n-1))$. $t = \frac{\bar{y}_1 - \bar{y}_2}{s\sqrt{\frac{2}{n}}}$. Reject H_0 if $|\bar{y}_1 - \bar{y}_2| \geq t_{\alpha/2}(2(n-1))\sqrt{\frac{2s^2}{n}}$, or $|\bar{y}_1 - \bar{y}_2| \geq t_{\alpha/2}(2(n-1))\sqrt{\frac{2MS(E)}{n}}$, Use $\alpha/2$ because H_a is two sided. The term $t_{\alpha/2}(2(n-1))\sqrt{\frac{2MS(E)}{n}}$ is called the *least significant difference(LSD).* It is the smallest value for which the significance between two means will be declared. This method of comparison between the means can be extended to certain cases of multi-parameters(i.e. more than two means).

case 1: Compare means of $p-1$ treatments with the mean of a control. Let μ_0 be the mean of the control. Let μ_1 be the mean of treatment 1, and so on. Let the means have a common variance, σ^2. Test $H_0 : \mu_i - \mu_0 = 0$, versus $H_a : \mu_i - \mu_0 \neq 0, i = 1, 2, ..., p-1$. **PROCEDURE:** Using the data, compute $\bar{y}_{0\cdot}, \bar{y}_{1\cdot}, ..., \bar{y}_{p-1\cdot}$ and the MS(E). Compute the LSD$= t_{\alpha/2}(p(r-1))\sqrt{\frac{2MS(E)}{r}}$. If $|\bar{y}_{i\cdot} - \bar{y}_{0\cdot}| > LSD$ for the i-th treatment, then the difference is significantly different from the control.

case 2: Consider an experiment where the treatments represent different levels of a factor. For example, doses of a medicine. In this setup, suppose we want to see whether increasing the levels give a higher yield. In this case, the LSD can be used. Let $\mu_1, \mu_2, ..., \mu_p$ be the means of the increasing treatment levels. Test $H_0 : \mu_i - \mu_{i+1} = 0$ versus $H_a : \mu_i = \mu_{i+1} \neq 0, i = 1, 2, ..., p-1$. Compute the LSD as $\sqrt{t_{\alpha/2}(p(r-1))\frac{2MS(E)}{r}}$. There is a significant difference if $|\bar{y}_{i\cdot} - \bar{y}_{i+1\cdot}| \geq LSD$.

8.3.2 Multiple Comparisons

If the problem is of pairwise comparisons of all the means, then the LSD method is not appropriate. Why? Let α be the required level of significance. The *Type I error* is defined as the probability of rejecting H_0 when H_0 is true. $1 - \alpha$ is the probability of accepting H_0 when H_0 is true. Suppose there are two comparisons, $(\mu_1, \mu_2), (\mu_1, \mu_3)$. Test $H_0 : \mu_1 - \mu_2 = 0$ and $H_0 : \mu_1 - \mu_3 = 0$. The probability of accepting both null hypotheses will be $(1-\alpha)^2$ assuming the tests are done independently. That is $P[|\bar{y}_{1\cdot} - \bar{y}_{2\cdot}| < LSD$ and $|\bar{y}_{1\cdot} - \bar{y}_{3\cdot}| < LSD] = (1-\alpha)^2$ assuming the two events are independent. The probability of rejecting H_0 is $1 - (1-\alpha)^2$. Hence, we need a method to keep α, the level of significance, for multiple comparisons fixed at the required level. Several methods are available:

1. *Fisher's protected LSD.* The SAS code is as follow:

```
PROC ANOVA;
CLASS TRT;
MODEL Y=TRT;
MEANS TRT/LSD;
```

2. *Tukey's Honestly significant difference.* The SAS code is as follow:

```
PROC ANOVA;
CLASS TRT;
MODEL Y=TRT;
MEANS TRT/TUKEY;
```

3. *Duncan's multiple range test.* The SAS code is as follow:

```
PROC ANOVA;
CLASS TRT;
MODEL Y=TRT;
MEANS TRT/DUNCAN;
```

4. *Student-Neumann-Keuls test.* The SAS code is as follow:

```
PROC ANOVA;
CLASS TRT;
MODEL Y=TRT;
MEANS TRT/SNK;
```

5. *Waller-Duncan Bayes LSD.* The SAS code is as follow:

```
PROC ANOVA;
CLASS TRT;
MODEL Y=TRT;
MEANS TRT/WALLER;
```

There are p population means, $\mu_1, \mu_2, ..., \mu_p$. Which of the pairs (μ_i, μ_j) are different?

Fisher's protected LSD Method The steps are as follow:

1. Use ANOVA table to test $H_0 : \mu_1 = \mu_2 = \cdots = \mu_p$. at α level of significance.
2. If H_0 is accepted then the procedure stops.
3. If H_0 is rejected, then compute $FPLSD = t_{\alpha/2}(p(r-1))\sqrt{\frac{2MS(E)}{n}}$ where r is the number of replications in each sample, $MS(E)$ is the mean square of error(pooled sample variance from p samples), and $p(r-1)$ is the degrees of freedom of the $MS(E)$.
4. If for any pair $(\bar{y}_{i\cdot}, \bar{y}_{j\cdot})$, the absolute difference $|\bar{y}_{i\cdot} - \bar{y}_{j\cdot}| \geq FPLSD$ then μ_i and μ_j are different. Do this for all possible pairs and determine the cluster of means. The previous SAS source code automatically tests at the $\alpha = 0.05$ significance level. To alter that, use

   ```
   MEANS TRT/LSD ALPHA=0.01
   ```

   to test at $\alpha = 0.01$ significance level.

Tukey's HSD Method the method is based on the distribution. The range is actually the studentized range. Let $\mu_1, \mu_2, ..., \mu_p$ be a random sample from $N(\mu, \sigma^2)$. Define the range $R = \max - \min$. The distribution of $Q = \frac{R}{s}$ is known and the cut-off points are tabulated.

1. For α, p and r, get $Q(\alpha, p, r)$ from the table of cutoff points of the distribution of the studentized range.
2. Compute $HSD = Q(\alpha, p, r)\sqrt{\frac{MS(E)}{r}}$.
3. For any pair $(\bar{y}_{i\cdot}, \bar{y}_{j\cdot})$, if $|\bar{y}_{i\cdot} - \bar{y}_{j\cdot}| \geq HSD$, then the difference $\mu_i - \mu_j$ is considered significant. Do this for all possible pairs.

SNK Method

1. Rank all p sample means from high to low.
2. Compute $SNK_i = Q(\alpha, i, r)\sqrt{\frac{MS(E)}{r}}, i = 2, 3, ..., p$.
3. If $|\bar{y}_h - \bar{y}_l| < SNK_p$ then no means are significant.
4. If $|\bar{y}_h - \bar{y}_l| \geq SNK_p$, then $\mu_h - \mu_l$ is significant. Next compare $|\bar{y}_h - \bar{y}_{l+1}|$ and $|\bar{y}_l - \bar{y}_{h-1}|$ with SNK_{p-1}.
5. Continue until all significant comparisons have been found.

8.4 Homework and Answers

1. An animal physiologist studied the pituitary function of hens put through a standard forced molt regimen used by egg producers to bring the hens back into egg production. Twenty-five hens were used for the study. Five hens were used for measurements at the premolt stage prior to the forced molt regimen and at the end of each of four stages of the forced molt regimen. The five stages of the regimen are (1) premolt (control), (2) fasting for 8 days, (3) 60 grams of Bran per day for 10 days, (4) 80 grams of Bran per day for 10 days, and (5) laying mash for 42 days. The objective was to follow various physiological responses associated with the pituitary function of the hens during the regimen to aid in explaining why the hens will come back into production after the forced molt. One of the compounds measured was serum T3 concentration. The data in the table are the serum T3 measurements for each of the five hens sacrificed at the end of each stage of the regimen.

Premolt	94.09	90.45	99.38	73.56	74.39
Fasting	98.81	103.55	115.23	129.06	117.61
60 g Bran	197.18	207.31	177.50	226.05	222.74
80 g Bran	102.93	117.51	119.92	112.01	101.10
Laying Mash	83.14	89.59	87.76	96.43	82.94

a. Write the linear statistical model for this study and explain the model components. A fixed means model with equal replication will be used to represent the data. Hens are being used as the subject, also called the experimental unit. There are 5 treatments (1) Premolt, (2) Fasting, (3) 60 g of Bran, (4) 80 g of Bran, and (5) Laying Mash. There are 5 replications per treatment. Thus, $p = 5$ and $r = 5$. The data can be summarized in the following format:

Summary of T3 Serum Format					
1	2	3	4	5	
$y_{1,1}$	$y_{2,1}$	$y_{3,1}$	$y_{4,1}$	$y_{5,1}$	
$y_{1,2}$	$y_{2,2}$	$y_{3,2}$	$y_{4,2}$	$y_{5,2}$	
$y_{1,3}$	$y_{2,3}$	$y_{3,3}$	$y_{4,3}$	$y_{5,3}$	
$y_{1,4}$	$y_{2,4}$	$y_{3,4}$	$y_{4,4}$	$y_{5,4}$	
$y_{1,5}$	$y_{2,5}$	$y_{3,5}$	$y_{4,5}$	$y_{5,5}$	Total

Substituting in the actual data yields the following chart:

Summary of T3 Serum Data						
	1	2	3	4	5	
	94.09	98.81	197.18	102.93	83.14	
	90.45	103.55	207.31	117.51	89.59	
	99.38	115.23	177.50	119.92	87.76	
	73.56	129.06	226.05	112.01	96.43	
	74.39	117.61	222.74	101.10	82.94	Total
Sum	431.87	564.26	1030.78	553.47	439.86	3020.24
Mean	86.374	112.852	206.156	110.694	87.972	604.048

The following equation will be used to determine the mean amount of T3 serum in the hens:

$$Y_{ij} = \mu_i + \epsilon_{ij}, i = 1, ..., 5; j = 1, ..., 5. \tag{8.1}$$

μ_i is the mean of the $i - th$ population. ϵ_{ij} is the experimental error. To obtain estimates of the means μ_i, the following equation will be used: $\hat{\mu}_i = \bar{Y}_{i\cdot} = \frac{1}{r}\sum_{j=1}^{r} Y_{ij}$. Hence, there will be 5 means computed as follow:

$$\hat{\mu}_1 = \bar{Y}_{1\cdot} = \frac{1}{5}\sum_{j=1}^{5} y_{1,j},\ \hat{\mu}_2 = \bar{Y}_{2\cdot} = \frac{1}{5}\sum_{j=1}^{5} y_{2,j},\ \hat{\mu}_3 = \bar{Y}_{3\cdot} = \frac{1}{5}\sum_{j=1}^{5} y_{3,j}$$

$$\hat{\mu}_4 = \bar{Y}_{4\cdot} = \frac{1}{5}\sum_{j=1}^{5} y_{4,j},\ \hat{\mu}_5 = \bar{Y}_{5\cdot} = \frac{1}{5}\sum_{j=1}^{5} y_{5,j}.$$

Referring back to equation (1), $\epsilon_{i,j}$, the error or variance, will be computed as follow: $\hat{\epsilon}_{ij} = y_{ij} - \hat{\mu}_i$. In the linear means model there will not be 5 variances or errors as there were 5 means. The variance is assumed to be the same for all replications. The following equation will be used to obtain the variance σ^2. $\hat{\sigma}^2 = \frac{1}{p(r-1)}\sum_{i=1}^{p}\sum_{j=1}^{r}(y_{ij} - \bar{y}_i)^2$. To summarize the above model, the means $\hat{\mu}_i$ are obtained with equation (2), and the variance is obtained with equation (4). An ANOVA Table will be used to analyze the variance. The ANOVA Table for the fixed means model with equal replication has the following format:

ANOVA Table Format

Source	d.f.	SS	MS
Treatment	$p-1$	$r\sum_{i=1}^{p}(y_{i\cdot}-\bar{y})^2$	$\frac{SST}{p-1}$
Error	$p(r-1)$	$\sum_{i=1}^{p}\sum_{j=1}^{r}(y_{i,j}-\bar{y}_{i\cdot})^2$	$\frac{SSE}{p(r-1)}$
Total	$rp-1$	$SST+SSE$	

b. State the assumptions necessary for an analysis of variance of the data. It is assumed that the data is Normally distributed. It is assumed that the data is an iid sequence, and that the populations have a common variance. It is assumed that the expected value of the error, $E(\epsilon)=0$, and the variance is $Var(\epsilon)=\sigma^2$.

c. Compute the analysis of variance for the data.

ANOVA Table for T3 Serum

Source	d.f.	SS	MS	F	p-value
Treatment	4	48568.8763	12142.219	78.08	0.0001
Error	20	3110.1892	155.509		
Total	24	51679.0655			

d. Compute the least square means and their standard errors for each treatment. Since the experiment is equi-replicated, the standard error is the same for all the means.

$$s_{\bar{y}}=\sqrt{\frac{s^2}{r}}=\sqrt{\frac{MSE}{r}}=\sqrt{\frac{155.509}{5}}=5.5769.$$

The means can be found in the table in part (a.).

e. Compute the 95% confidence interval estimates of the treatment means.

$$\bar{y}_1\pm t_{0.025}\sqrt{\frac{MSE}{5}}=86.374\pm(2.776)\sqrt{\frac{155.509}{5}}=86.374\pm 15.481=[70.89,101.86].$$

$$\bar{y}_2\pm t_{0.025}\sqrt{\frac{MSE}{5}}=112.852\pm(2.776)\sqrt{\frac{155.509}{5}}=112.852\pm 15.481=[97.371,128.333].$$

$$\bar{y}_3\pm t_{0.025}\sqrt{\frac{MSE}{5}}=206.156\pm(2.776)\sqrt{\frac{155.509}{5}}=206.156\pm 15.481=[190.675,221.637].$$

$$\bar{y}_4\pm t_{0.025}\sqrt{\frac{MSE}{5}}=110.694\pm(2.776)\sqrt{\frac{155.509}{5}}=110.694\pm 15.481=[95.213,126.175].$$

$$\bar{y}_5\pm t_{0.025}\sqrt{\frac{MSE}{5}}=87.972\pm(2.776)\sqrt{\frac{155.509}{5}}=87.972\pm 15.481=[72.491,103.453].$$

f. Test the hypothesis of no differences among means of the five treatments with the F test at the 0.05 level of significance. The hypothesis being tested is stated as follow: $H_0:\mu_1=\mu_2=\mu_3=\mu_4=\mu_5$. $H_a:\mu_i\neq\mu_j, i\neq j, i\in 1..5, j\in 1..5$. $F_{0.05(4,20)}=2.87$. Since $78.08>2.87$, the differences among means is significant.

2. Consider the experiment in Exercise 1. Suppose some of the chickens were lost during the course of the experiment resulting in the following set of observations.

Premolt	94.09	90.45	99.38	73.56	
Fasting	98.81	103.55	115.23	129.06	117.61
60 g Bran	197.18	207.31	177.50		
80 g Bran	102.93	117.51	119.92	112.01	101.10
Laying Mash	82.94	83.14	89.59	87.76	

a. Write the linear statistical model for this study and explain the model components. A fixed means model with unequal replication will be used to represent the data. There are still 5 treatments. Thus, $p = 5$. However, the replications for each experiment have changed. So, r will have to be defined for each treatment. r_1 will be used for the Premolt treatment, r_2 will be used for the Fasting treatment, r_3 will be used for the 60 g of Bran treatment, r_4 will be used for the 80 g of Bran treatment, and r_5 will be used for the Laying mash treatment. From the given data, it can be seen that $r_1 = 4$, $r_2 = 5$, $r_3 = 3$, $r_4 = 5$, and $r_5 = 4$. The data is put into the following tabular format:

Summary of T3 Serum Format

1	2	3	4	5	
$y_{1,1}$	$y_{2,1}$	$y_{3,1}$	$y_{4,1}$	$y_{5,1}$	
$y_{1,2}$	$y_{2,2}$	$y_{3,2}$	$y_{4,2}$	$y_{5,2}$	
$y_{1,3}$	$y_{2,3}$	$y_{3,3}$	$y_{4,3}$	$y_{5,3}$	
$y_{1,4}$	$y_{2,4}$		$y_{4,4}$	$y_{5,4}$	
	$y_{2,5}$		$y_{4,5}$		Total

Substituting in the actual data yields the following chart:

Summary of T3 Serum Data

	1	2	3	4	5	
	94.09	98.81	197.18	102.93	82.94	
	90.45	103.55	207.31	117.51	83.14	
	99.38	115.23	177.50	119.92	87.76	
	73.56	129.06		112.01	87.76	
		117.61		101.10		Total
Sum	357.48	564.26	581.99	553.47	343.43	2400.63
Mean	89.37	112.852	194.00	110.694	85.858	592.774

The main equation is as follow: $Y_{i,j} = \mu_i + \epsilon_{i,j}, j = 1, ..., r_i, i = 1, ..., p$. The estimators of the model are as follow: $\hat{\mu}_i = \bar{y}_i = \frac{1}{r_i}\sum_{j=1}^{r_i} y_{i,j}, i \in 1..5$. $\hat{\mu}$ is the average of T3 serum as before. Hence, there will be 5 means computed as follow:

$$\hat{\mu}_1 = \bar{Y}_{1\cdot} = \frac{1}{4}\sum_{j=1}^{4} y_{1,j},\ \hat{\mu}_2 = \bar{Y}_{2\cdot} = \frac{1}{5}\sum_{j=1}^{5} y_{2,j},\ \hat{\mu}_3 = \bar{Y}_{3\cdot} = \frac{1}{3}\sum_{j=1}^{3} y_{3,j}$$

$$\hat{\mu}_4 = \bar{Y}_{4\cdot} = \frac{1}{5}\sum_{j=1}^{5} y_{4,j},\ \hat{\mu}_5 = \bar{Y}_{5\cdot} = \frac{1}{4}\sum_{j=1}^{4} y_{5,j}.$$

Referring back to equation (5), the variance or error of each piece of data is expressed as follow: $SE(\hat{\mu}_i) = \frac{s}{\sqrt{r_i}}, i = 1, ..., p$. The standard error is the variance of the data as before. There will be a standard error for each treatment instead of a common σ^2. Essentially, in this model, r_i is used for each treatment instead of a common r. The ANOVA Table will still be used to analyze the variance. However, the formulas will have a slightly different form. The ANOVA Table for the means model with unequal replications follows.

ANOVA Table Format

Source	d.f.	SS	MS
Treatment	$p-1$	$\sum_{i=1}^{p} r_i(y_{i\cdot} - \bar{y})^2$	$\frac{SST}{p-1}$
Error	$\sum_{i=1}^{p} r_i - p$	$\sum_{i=1}^{p}\sum_{j=1}^{r_i}(y_{i,j} - \bar{y}_{i\cdot})^2$	
Total	$\sum_{i=1}^{p} r_i - 1$	$SST + SSE$	

b. State the assumptions necessary for an analysis of the data. It is assumed that the data is an iid sequence and Normally distributed. It is assumed that the expected value of the error $E(\epsilon) = 0$.

c. Compute the analysis of variance for the data.

ANOVA Table for T3 Serum

Source	d.f.	SS	MS	F	p-value
Treatment	4	24852.093	6213.023	57.565	0.0001
Error	16	1726.897	107.931		
Total	20	26578.99			

d. Compute the least squares means and their standard errors for each treatment. How has the loss of some chickens from the experiment affected the estimates of the means? By comparing the individual means for each treatment, it can be seen that the mean of treatment 1 increased. The means for treatments 3 and 5 decreased. The means of treatments 2 and 4 remain unchanged since no hens were lost during treatment. The over-all mean of the experiment decreased due to the loss of hens. The actual means can be found in part (a). The standard errors are as follow:

1. For the mean of treatment 1,
$$s_{\bar{y}} = \sqrt{\frac{MSE}{r_1}} = \sqrt{\frac{107.931}{4}} = 5.1945.$$
2. For the mean of treatment 2,
$$s_{\bar{y}} = \sqrt{\frac{MSE}{r_2}} = \sqrt{\frac{107.931}{5}} = 4.646.$$
3. For the mean of treatment 3,
$$s_{\bar{y}} = \sqrt{\frac{MSE}{r_3}} = \sqrt{\frac{107.931}{3}} = 5.998.$$
4. For the mean of treatment 4,
$$s_{\bar{y}} = \sqrt{\frac{MSE}{r_4}} = \sqrt{\frac{107.931}{5}} = 4.646.$$
5. For the mean of treatment 5,
$$s_{\bar{y}} = \sqrt{\frac{MSE}{r_5}} = \sqrt{\frac{107.931}{4}} = 5.1945.$$

e. Compute the 95% confidence interval estimates of the treatment means.

$$\bar{y}_1 \pm t_{0.025}\sqrt{\frac{MSE}{4}} = 89.37 \pm (2.776)\sqrt{\frac{107.931}{4}} = 89.37 \pm 14.42 = [74.95, 103.79].$$

$$\bar{y}_2 \pm t_{0.025}\sqrt{\frac{MSE}{5}} = 112.852 \pm (2.776)\sqrt{\frac{107.931}{5}} = 112.852 \pm 12.898 = [99.95, 125.75].$$

$$\bar{y}_3 \pm t_{0.025}\sqrt{\frac{MSE}{3}} = 194.00 \pm (2.776)\sqrt{\frac{107.931}{3}} = 194.00 \pm 16.65 = [177.35, 210.65].$$

$$\bar{y}_4 \pm t_{0.025}\sqrt{\frac{MSE}{5}} = 110.694 \pm (2.776)\sqrt{\frac{107.931}{5}} = 110.694 \pm 12.898 = [97.796, 123.592].$$

$$\bar{y}_5 \pm t_{0.025}\sqrt{\frac{MSE}{4}} = 85.858 \pm (2.776)\sqrt{\frac{107.931}{4}} = 85.858 \pm 14.42 = [71.438, 100.278].$$

f. Test the hypothesis of no differences among means of the five treatments with the F test at the 0.05 level of significance. The hypothesis being tested is stated as follow: $H_0 : \mu_1 = \mu_2 = \mu_3 = \mu_4 = \mu_5$. $H_a : \mu_i \neq \mu_j, i \neq j, i \in 1..5, j \in 1..5$. $F_{0.05(4,16)} = 3.01$. Since $57.565 > 3.01$, the differences among means is significant.

3. Contrasts of interest are the serum T3 concentration differences between successive stages(use the equally replicated data).

(a) Estimate each of the contrasts and their standard deviations. To estimate each pairwise contrast, the following equation will be used: $\hat{\theta} = \sum_{i=1}^{p} k_i \bar{y}_{i\cdot}$, subject to the condition that $\sum_{i=1}^{p} k_i = 0$. That produces the following 4 expressions. $\hat{\theta}_1 = \bar{y}_{1\cdot} - \bar{y}_{2\cdot} = -26.478$. $\hat{\theta}_2 = \bar{y}_{2\cdot} - \bar{y}_{3\cdot} = -11.83$. $\hat{\theta}_3 = \bar{y}_{3\cdot} - \bar{y}_{4\cdot} = 12.10$. $\hat{\theta}_4 = \bar{y}_{4\cdot} - \bar{y}_{5\cdot} = 2.88$. To estimate the standard deviation of each pairwise contrast, the following equation will be used:

$$SE(\hat{\theta}) = \frac{s}{\sqrt{r}}\sqrt{\sum_{i=1}^{p} k_i^2}. \tag{8.2}$$

The standard error for each pairwise contrast will be the same since the same number of replications have been performed. $SE(\hat{\theta}_i) = \frac{s}{\sqrt{5}}\sqrt{2} = 7.88693745, i \in 1,..,4$.

(b) Test for significance of the contrasts using F-tests. The F value is calculated with the following formula: $F = \frac{SSC}{MSE}$. To find the theoretical F statistic in a table, one more parameter is needed. The level of significance denoted by α. For $\theta_1 : H_0 : \theta_1 = 0$. $H_a : \theta_1 \neq 0$. $F_{1,20} = 4.35$ for $\alpha = 0.05$. Since, $11.27 > 4.35$, H_0 is rejected. Also, the p-value of the contrast is very small. For θ_2 : $H_0 : \theta_2 = 0$. $H_a : \theta_2 \neq 0$. Using the same arbitrarily set significance level as in the above test, since $139.95 > 4.35$, the H_0 hypothesis is rejected. For $\theta_3 : H_0 : \theta_3 = 0$. $H_a : \theta_3 \neq 0$. Since $146.5 > 4.35$, reject H_0. For $\theta_4 : H_0 : \theta_4 = 0$. $H_a : \theta_4 \neq 0$. Since $8.30 > 4.35$, reject H_0. The calculated F values can be found at the end in the contrast table.

3. Use multiple comparison methods for analyzing serum T3 concentration data using the following 3 methods: LSD, HSD, SNK.

LSD: The LSD(Least Significant Difference) is used to compare multiple means among multiple treatments. The LSD statistic is calculated as follow: $LSD = \sqrt{\frac{2MSE}{r}} t_{\alpha/2,p(r-1)} = \sqrt{\frac{2(155.5095)}{5}}(2.086) =$ 16.452 So, whenever the difference of two means differ by more than 16.452, it is said that the two means is significantly different. From reading the SAS printout, it can be seen that Treatment 3 is significantly different from Treatments 2, 4, 5, 1. Treatment 2 is significantly different from Treatments 3, 5, 1. Treatment 4 is significantly different from Treatments 3, 5, 1. Treatment 5 is significantly different from Treatments 3, 2, 4. And Treatment 1 is significantly different from Treatments 3, 2, 4. However, Treatment 2 is not significantly different from Treatment 4, and Treatment 5 is not significantly different from treatment 1.

HSD: To compute Tukey's HSD(Honest Significant Difference), the following equation will be used: $HSD = Q(\alpha, p, p(r-1))\sqrt{\frac{MSE}{r}}$. Thus, $HSD = 4.232\sqrt{\frac{155.5095}{5}} = 23.601$. For any difference in means that is greater than 23.601, the difference will be considered to be significant. Observing the SAS printout, it can be seen that Treatment 3 is significantly different from Treatments 2, 4, 5, 1. Treatment 2 is significantly different from Treatments 3, 5, 1. Treatment 4 is significantly different from Treatments 3, 2, 5, 1. Treatment 5 is significantly different from Treatments 3, 2, 4. Treatment 1 is significantly different from Treatments 3, 2, 4. However, Treatment 2 is not significantly different from Treatment 4, and Treatment 5 is not significantly different from Treatment 1.

SNK: To calculate the SNK statistic, the following equation will be used: $SNK_i = Q(\alpha, i, p(r-1))\sqrt{\frac{MSE}{r}}, i \in 2, 3, 4, 5$. Thus, $SNK_2 = 2.95\sqrt{\frac{155.5095}{5}} = 16.451867$. $SNK_3 = 3.58\sqrt{\frac{155.5095}{5}} = 19.95381$. $SNK_4 = 3.96\sqrt{\frac{155.5095}{5}} = 22.075044$. $SNK_5 = 4.232\sqrt{\frac{155.5095}{5}} = 23.600681$. Whenever the difference of two means is greater for each SNK value of each treatment, the difference is considered significant. From observing the SAS printout, it can be seen that Treatment 3 is significantly different from Treatments 2, 4, 5, 1. Treatment 2 is significantly different from Treatments 3, 5, 1. Treatment 4 is significantly different from Treatments 3, 5, 1. Treatment 5 is significantly different from Treatments 3, 2, 4. Treatment 1 is significantly different from Treatments 3, 2, 4. However, Treatment 2 is not significantly different from Treatment 4, and Treatment 5 is not significantly different from Treatment 1.

8.5 Random Effects Model

In the 1-way ANOVA model(also called a fixed effects model), the p treatments are fixed. There are cases where the p treatments are not fixed but are drawn randomly from a population of treatments.

Example: In a manufacturing environment, suppose a large number of machines. The problem is to study the variation from one machine to another. For this problem, p machines from the pool of machines are randomly selected for the study. Each machine is a treatment as before.

The model statement for a random effects model is $y_{ij} = \mu_i + \epsilon_{ij}, i = 1, 2, ..., p; j = 1, 2, ..., r$. The assumptions are

1. $\epsilon_{ij} \sim N(0, \sigma^2)$.
2. $\mu_i \sim N(\mu, \sigma^2_\tau)$.
3. ϵ_{ij} and μ_i are independent.

Another form of the random effects model is $y_{ij} = \mu + \tau_i + \epsilon_{ij}$, where $\tau_i \sim N(0, \sigma^2_\tau)$, and $\epsilon_{ij} \sim N(0, \sigma^2_\tau)$. Problems of interest include:

1. Test $H_0 : \sigma^2_\tau = 0$, versus $H_a : \sigma^2_\tau > 0$.
2. Estimate σ^2_τ.

Construct an ANOVA table as in the fixed effects model. Under the random effects model, $E(MS(E)) = \sigma^2$, and $E(MS(TRT)) = \sigma^2 + r\sigma^2_\tau$. If the F statistic is small, then accept H_0. If F is large then reject H_0. An estimate of the treatment variation is given by $\hat{\sigma}^2_\tau = \frac{MS(TRT) - MS(E)}{r}$ which is an unbiased estimate of the variance.

Example: A plant pathologist took 4 3-paired samples from 5-ton lots of cotton seed, accumulated at various cotton gins during the ginning season. The data of aflation concentrations in foots per billion is given:

Lot no.	Afflation
L1	39, 57, 63, 66
L2	56, 13, 25, 31
L3	64, 83, 88, 71
L4	29, 55, 21, 51
L5	39, 66, 53, 81
L6	11, 49, 34, 10
L7	23, 0, 5, 20
L8	10, 11, 23, 37

The model statement is $y_{ij} = \mu_i + \epsilon_{ij}, i = 1, 2, ..., 8, j = 1, 2, ...4$. The assumptions of this model are as follow:

1. $\mu_i \sim N(0, \sigma_\tau^2$.
2. $\epsilon_{ij} \sim N(0, \sigma^2)$.

The partial SAS code is

```
...
INPUT LOT Y;
...


PROC GLM;
CLASS LOT;
MODEL Y=LOT;
RANDOM LOT/TEST;
RUN;
```

The ANOVA table produced is

Source	d.f.	SS	MS	F	p-value
Lots	7	13696.47	1956.64	8.46	0.0001
Error	24	5548.25	231.18		
Total	31	19244.72			

The F-statistic is used to test $H_0 : \sigma_\tau^2 = 0$ versus $H_a : \sigma_\tau^2 > 0$. Since the p-value of 0.0001 is far less than $\alpha = 0.01$, reject the null hypothesis. Let's estimate the variance components. The components are σ_τ^2 and σ^2. $\hat{\sigma}^2 = MS(E) = 231.18$. $\hat{\sigma}_\tau^2 = \frac{MS(TRT) - MS(E)}{r} = \frac{1956.64 - 231.18}{4} = 431.65$. The lot expected mean squares is $Var(Error) + 4Var(Lot)$. Recall that $E(MS(E)) = \sigma^2$. $E(MS(TRT)) = \sigma^2 + r\sigma_\tau^2$. The *intra-class correlation coefficient* is given by $\rho = \frac{\sigma_\tau^2}{\sigma^2 + \sigma_\tau^2} = 0.65$.

8.6 CRD with Nesting

Such models are also called two stage nested or hierarchical designs. See Figure 8.3.

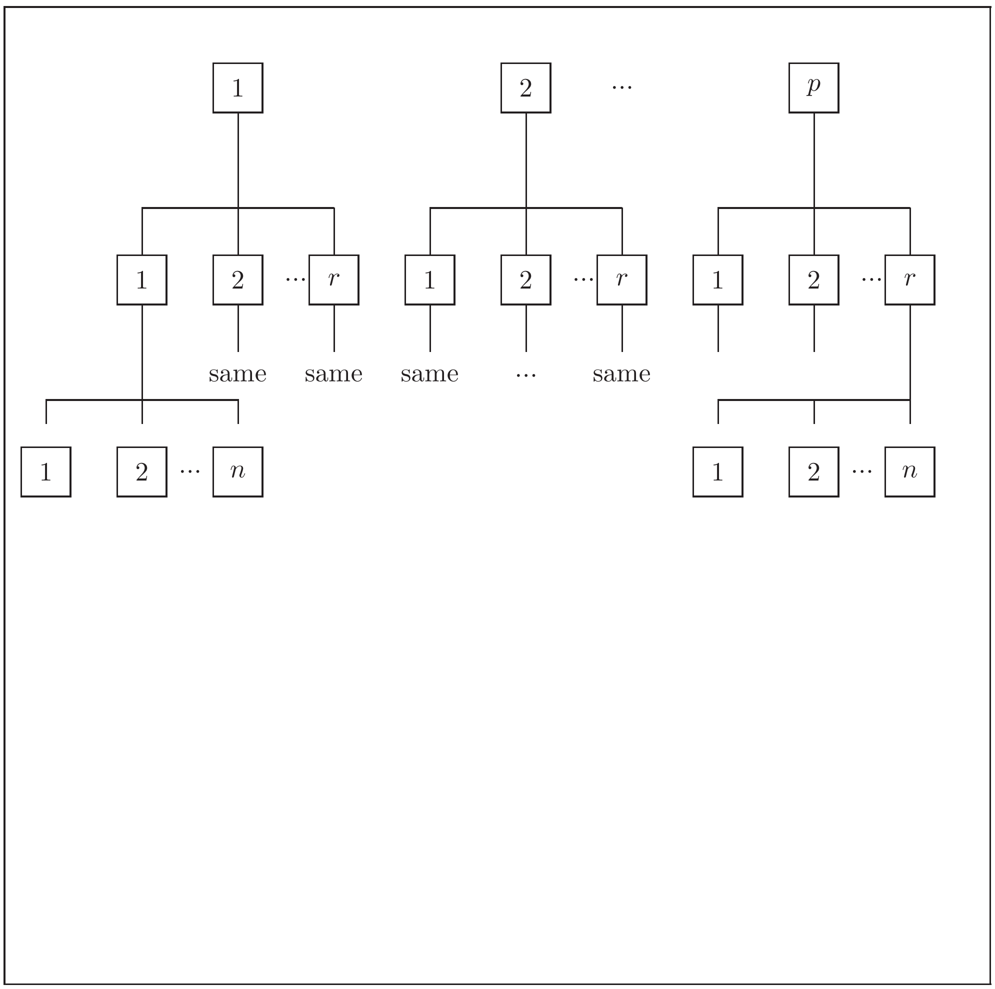

Figure 8.3:

Example: A soil scientist studied the growth of barley plants under three different levels of salinity. There were 2 replicate containers for each treatment, in a completely randomized design. Three plants were measured in each replication. The factor is salinity with three levels 1) control, 2) 6 bars, 3) 12 bars. Thus, $p = 3$, $r = 2$ and $n = 3$.

Example: A company purchases its raw material from three different suppliers. Each supplier delivers material in 4 batches. To test the purity of the material, 3 samples from each of the 4 batches were considered. $p = 3$, $r = 4$ and $n = 3$.

The nested design model statement is $y_{ijk} = \mu_i + \delta_{ijk} + \epsilon_{ij}, i = 1, 2, ..., p, j = 1, 2, ..., r, k = 1, 2, ...n$. y_{ijk} is the yield. ϵ_{ij} is the variation of the j-th experimental unit on the i-th treatment. δ_{ijk} is the random variation of the k-th sampling unit from the j-th experimental unit on the i-th treatment. $\sigma^2 = Var(\epsilon_{ij})$ which is the variation of the error or the measure of the variation in the experimental units. The two sources of variation in the experimental error are:

1. Variation among the experimental units on the same treatment.
2. Variation among the sampling units within experimental units.

The assumptions of the model are:

1. $\epsilon_{ij} \sim N(0, \sigma^2_\epsilon)$.
2. $\delta_{ijk} \sim N(0, \sigma^2_\delta)$.

The decomposition of the total sums of squares is $\sum_{i=1}^p \sum_{j=1}^r \sum_{k=1}^n (y_{ijk} - \bar{y})^2$, where $\bar{y} = \frac{1}{npr} \sum_{i=1}^p \sum_{j=1}^r \sum_{k=1}^n y_{ijk}$. In the previous example, $\bar{y}_{11\cdot} = \frac{1}{3} \sum_{k=1}^3 y_{11k}$, for each experimental unit. $\bar{y}_{1\cdot\cdot}$ for each treatment. The total sum of squares can be rewritten as

$$\sum_{i=1}^p \sum_{j=1}^r \sum_{k=1}^n (y_{ijk} - \bar{y}_{ij\cdot} + \bar{y}_{ij\cdot} - \bar{y}_{i\cdot\cdot} + \bar{y}_{i\cdot\cdot} - \bar{y})^2 =$$

$$\overbrace{\sum_{i=1}^p \sum_{j=1}^r \sum_{k=1}^n (y_{ijk} - \bar{y}_{ij\cdot})^2}^{SS(SAMPLING)} + \overbrace{n \sum_{i=1}^p \sum_{j=1}^r (\bar{y}_{ij\cdot} - \bar{y}_{i\cdot\cdot})^2}^{SS(E)} + \overbrace{nr \sum_{i=1}^p (\bar{y}_{i\cdot\cdot} - \bar{y})^2}^{SS(TRT)}.$$

The cross product terms sum to zero to get, $SS(SAMPLING) + SS(E) + SS(TRT)$. The general ANOVA table is as follow:

Source	d.f.	SS	MS
Treatment	$p - 1$	SS(TRT)	$\frac{SS(TRT)}{p-1}$
Experimental Error	$p(r - 1)$	SS(E)	$\frac{SS(E)}{p(r-1)}$
Sampling Error	$pr(n - 1)$	SS(SMPLNG)	$\frac{SS(SMPLNG)}{pr(n-1)}$
Total	$npr - 1$	SS(TOTAL)	

The expected values of the mean squares are as follow: $E(MS(TRT)) = \sigma^2_\delta + n\sigma^2_\epsilon + \frac{rn}{p-1} \sum_{i=1}^p (\mu_i - \bar{\mu})^2$, where $\bar{\mu} = \frac{1}{p} \sum_{i=1}^p \mu_i$, $E(MS(E)) = \sigma^2_\delta + n\sigma^2_\epsilon$, $E(MS(SAMPLING)) = \sigma^2_\delta$. The hypotheses tests are as follow: $F_1 = \frac{MS(TRT)}{MS(E)} \sim F(p-1, p(r-1))$, for $H_0 : \mu_1 = \mu_2 = \cdots = \mu_p$. $F_2 = \frac{MS(E)}{MS(SAMPLING)} \sim F(p(r-1), rp(n-1))$, for $H_0 : \sigma^2_\epsilon = 0$. The estimation of the variance components is as follow: $\hat{\sigma}^2_\delta = MS(SAMPLING)$ and $\hat{\sigma}^2_\epsilon = \frac{MS(E) - MS(SAMPLING)}{n}$. Some SAS code to produce the ANOVA table is as follow:

```
DATA A;
INPUT MANUF & FILLER & Y;
CARDS;
1 1 0.12
1 1 1.10
...
2 3 1.58
...

PROC GLM;
CLASSES MANUF FILLER;
MODEL Y=MANUF FILLER(MANUF);
RANDOM FILLER(MANUF)/TEST;
RUN;
```

Note that the `TEST` statement ensures the correct ratios for the hypotheses tests are used.

8.7 Two-stage Nested Design

There are p treatments and rp experimental units. The data can be arranged in the same way as the 1-way nested design. The model statement is $y_{ijk} = \mu_i + \epsilon_{ij} + \delta_{ijk}$. y_{ijk} is the observation in the k-th sampling unit in the j-th experimental unit treated with the i-th treatment. $\epsilon_{ij} \sim N(0, \sigma_\epsilon^2)$. $\delta_{ijk} \sim N(0, \sigma_\delta^2)$. The ANOVA table is similar to the previous nested design ANOVA table.

Source	d.f.	SS	MS	E(MS)
Trt	$p-1$	$SS(TRT)$	$\frac{SS(TRT)}{p-1}$	$\sigma_\delta^2 + r\sigma_\epsilon^2 + \frac{rn}{p-1}\sum(\mu_i - \mu)^2$
Exp error	$p(r-1)$	$SS(E)$	$\frac{SS(E)}{p(r-1)}$	$\sigma_\delta^2 + \sigma_\epsilon^2$
Smp error	$pr(n-1)$	$SS(SMP)$	$\frac{SS(SMP)}{pr(n-1)}$	σ_δ^2
Total	$npr-1$			

$F_1 = \frac{MS(TRT)}{MS(E)} \sim F(p-1, p(r-1))$. $F_2 = \frac{MS(E)}{MS(SAMPLING)} \sim F(p(r-1), rp(n-1))$. The hypotheses tests are as follow: $H_0 : \mu_1 = \mu_2 = \cdots = \mu_p$. $H_a : \mu_i \neq \mu_j$, for at least one (i, j) pair. Use the F_1 statistic. The other hypothesis test is $H_0 : \sigma_\epsilon^2 = 0$. $H_a : \sigma_\epsilon^2 > 0$. Use the F_2 statistic. If H_0 in F_2 is rejected, then H_0 in F_1 will probably be rejected. The nested designs are commonly used when the nesting is another factor (not necessarily in the sense of experimental and sampling units). The *fixed effects nested model* is given by: $y_{ijk} = \mu_i + \beta_{ij} + \epsilon_{ijk}$. μ_i is the effect of the i-th level of the main factor. β_{ij} is the effect of the j-th level of the nested factor in the i-th level of the main factor. ϵ_{ijk} is the random error and is $N(0, \sigma^2)$. The same ANOVA table is used as before, but the last two columns are different. $E(MS(TRT)) = \sigma^2 + \frac{rn}{p-1}\sum_{i=1}^{p}(\mu_i - \bar{\mu})^2$. $F_1 = \frac{MS(TRT)}{MS(E)} \sim F(p-1, p(r-1))$. $E(MS(NESTING)) = \sigma^2 + \frac{n}{p(r-1)}\sum_i\sum_j(\beta_{ij} - \bar{\beta}_{i\cdot})^2$. $F_2 = \frac{MS(NESTING)}{MS(E)} \sim F(p(r-1), rp(n-1))$. $MS(NESTING)$ is $MS(E)$ in the previous table. $E(MS(E)) = \sigma^2$. $MS(E)$ is $MS(SAMPLING)$ in the previous table. The hypotheses tests are as follow: $H_0 : \mu_1 = \mu_2 = \cdots = \mu_p$. $H_a : \mu_i \neq \mu_j$. Use the F_1 statistic. $H_0 : \beta_{i1} = \beta_{i2} = \cdots = \beta_{ir}, i \in 1, 2, ..., p$. $H_a : \beta_{ij} \neq \beta ik, j, k \in 1, 2, ..., r$. Use the F_2 statistic. In the fixed effects model:

1. μ_i is the fixed main factor.
2. β_{ij} is the fixed nested factor.
3. ϵ_{ijk} is the random error.

In a *mixed effects model:* Use the same model statement, but

1. μ_i is the fixed main factor.

2. β_{ij} is the random nested factor and is $N(0, \sigma_\beta^2)$.

3. ϵ_{ijk} is the random error and is $N(0, \sigma^2)$.

In a *random effects model:* Use the same model statement, but

1. μ_i is the randomized main factor and is $N(0, \sigma_\mu^2)$.

2. β_{ij} is the random nested factor and is $N(0, \sigma_\beta^2)$.

3. ϵ_{ijk} is the random error and is $N(0, \sigma^2)$.

The sums of squares for the first nested model are as follow: $SS(TRT) = nr\sum_{i=1}^p(\bar{y}_{i\cdot\cdot} - \bar{y})^2$. $SS(NESTING) = n\sum_{i=1}^p\sum_{j=1}^r(\bar{y}_{ij\cdot} - \bar{y}_{i\cdot\cdot})^2$. $SS(E) = \sum_{i=1}^p\sum_{j=1}^r\sum_{k=1}^n(y_{ijk} - \bar{y}_{ij\cdot})^2$. $SS(TOTAL) = \sum_{i=1}^p\sum_{j=1}^r\sum_{k=1}^n(y_{ijk} - \bar{y})^2$. When μ is fixed and β is fixed, $E(MS(TRT)) = \sigma^2 + \frac{np}{p-1}\sum_{i=1}^p(\mu_i - \bar{\mu})^2$. $E(MS(NESTING)) = \sigma^2 + \frac{n}{p(r-1)}\sum_{i=1}^p\sum_{j=1}^r(\beta_{ij} - \bar{\beta}_{i\cdot})^2$. $E(MS(E)) = \sigma^2$. The SAS code that produces those expected values is as follow:

```
PROC GLM;
CLASS TRT NEST;
MODEL Y=TRT NEST(TRT);
RUN;
```

When μ is fixed and β is random, $E(MS(TRT)) = \sigma^2 + n\sigma_\beta^2 + \frac{rn}{p-1}\sum_{i=1}^p(\mu_i - \bar{\mu})^2$. $E(MS(NESTING)) = \sigma^2 + n\sigma_\beta^2$. $E(MS(E)) = \sigma^2$. The SAS source code is

```
PROC GLM;
CLASS TRT NEST;
MODEL Y=TRT NEST(TRT);
RANDOM NEST(TRT)/TEST;
```

When μ is random and β is random, $E(MS(TRT)) = \sigma^2 + n\sigma_\beta^2 + nr\sigma_\mu^2$. $E(MS(NESTING)) = \sigma^2 + n\sigma_\beta^2$. $E(MS(E)) = \sigma^2$. The SAS source code is

```
PROC GLM;
CLASS TRT NEST;
MODEL Y=TRT NEST(TRT);
RANDOM TRT NEST(TRT)/TEST;
```

8.8 Randomized Block Design(RBD)

There are p treatments. From rp experimental units, form r homogeneous groups called *blocks.* A randomized block design for p treatments each replicated r times is constructed as follow:

- First group the experimental units into r blocks of p units each in such a way that the units within blocks are as nearly alike as possible.

- Then assign at random the treatments to the units within the blocks subjected to the restriction that each treatment occurs only once in each block.

- Blocks must be selected so that the variance among units within blocks is smaller than the variance over the whole set of units.

In the end, there will be r blocks of size p.

Example: Consider the following design: 3 blocks and 4 treatments.

A	B	C	D
B	C	D	A
C	D	A	B

The data can be put into the following general format:

Blocks	1	...	p	Row means
1	y_{11}	...	y_{1p}	$\bar{y}_{1\cdot}$
2	y_{21}	...	y_{2p}	$\bar{y}_{2\cdot}$
3	y_{31}	...	y_{3p}	$\bar{y}_{3\cdot}$
.	.	...	.	.
.	.	...	.	.
.	.	...	.	.
r	y_{r1}	...	y_{rp}	$\bar{y}_{r\cdot}$
	$\bar{y}_{\cdot 1}$	...	$\bar{y}_{\cdot p}$	$\bar{y}_{\cdot\cdot}$

The model statement is as follow: $y_{ij} = \mu + \tau_j + \beta_i + \epsilon_{ij}, i = 1, 2, ..., r; j = 1, 2, ..., p$. y_{ij} is the yield in the i-th block when the j-th treatment is used. μ is the overall mean. τ_j is the effect of the j-th treatment. β_i is the effect of the i-th block. ϵ_{ij} is the random error and is $N(0, \sigma^2)$. The sums of squares are given as follow:

$$SS(TOTAL) = \sum_i \sum_j (y_{ij} - \bar{y})^2 = \sum_i \sum_j (y_{ij} - \bar{y}_{\cdot j} - \bar{y}_{i\cdot} + \bar{y} + \bar{y}_{\cdot j} - \bar{y} + \bar{y}_{i\cdot} - \bar{y})^2 =$$

$$\overbrace{r \sum_{j=1}^{p} (\bar{y}_{\cdot j} - \bar{y})^2}^{\text{SS(TRT)}} + \overbrace{p \sum_{i=1}^{r} (\bar{y}_{i\cdot} - \bar{y})^2}^{\text{SS(BLOCK)}} + \overbrace{\sum_{i=1}^{r} \sum_{j=1}^{p} (y_{ij} - \bar{y}_{i\cdot} - \bar{y}_{\cdot j} + \bar{y})^2}^{\text{SS(E)}}.$$

The ANOVA table is as follow:

Source	d.f.	SS	MS
Treatment	$p-1$	SS(TRT)	MS(TRT)
Block	$r-1$	SS(BLOCK)	MS(BLOCK)
Error	$(r-1)(p-1)$	SS(E)	MS(E)
Total	$pr-1$	SS(TOTAL)	

Problems of interest:

1. Test $H_0 : \tau_1 = \tau_2 = \cdots = \tau_p$, or test $H_0 : \sigma^2_\tau = 0$ if a random effects model is used. Under H_0, $F_1 \sim F(p-1, (p-1)(r-1))$. Hence, the test can be performed.

2. Check whether blocking is effective. If $F_2 > 1$, then blocking is effective. Also, the *relative efficiency* is defined as $RE = \frac{(r-1)MS(BLOCK)+r(p-1)MS(E)}{(rp-1)MS(E)}$. If $RE > 1$, then blocking is effective. But, $RE > 1 \Leftrightarrow F_2 > 1$, $RE < 1 \Leftrightarrow F_2 < 1$, and $RE = 1 \Leftrightarrow F_2 = 1$. Thus, one or the other method of testing the null hypothesis can be used.

3. Estimate the means. The mean of the j-th treatment is $\mu + \tau_j, j = 1, 2, ..., p$. The least squares estimator of

8.8.1 Confidence Interval of $(\tau_j - \tau_{j'})$

Note that $(\tau_j - \tau_{j'}) = (\mu + \tau_j) - (\mu + \tau_{j'})$. Hence, an estimate of $\tau_j - \tau_{j'}$ is $\bar{y}_{\cdot j} - \bar{y}_{\cdot j'}$. The standard error is $\sqrt{\frac{2MS(E)}{r}}$. A 100% confidence interval for $\tau_j - \tau_{j'}$ is $\bar{y}_{\cdot j} - \bar{y}_{\cdot j'} \pm t_{\alpha/2}((r-1)(r-1))\sqrt{\frac{2MS(E)}{r}}$.

Example: Hardness testing experiment. There are four methods of testing the hardness of a metal. There are four different metals used as blocks. Cut each metal into four sections. The data is as follow:

	1	2	3	4
1	9.3	9.4	9.2	9.7
2	9.4	9.3	9.4	9.6
3	9.6	9.8	9.5	10
4	10	9.9	9.7	10.2

The SAS source code to generate the ANOVA table is as follow:

```
DATA A;
INPUT TRT $ BLOCK $ Y;
CARDS;
1 1 9.3
1 2 9.4
1 3 9.6
1 4 10
...


PROC ANOVA;
CLASSES TRT BLOCK;
MODEL Y=TRT BLOCK;
RUN;
```

The ANOVA table produced appears like this:

Source	d.f	SS	MS	F	p-value
Treatment	3	0.385	0.128	14.44	0.0009
Block	3	0.825	0.275	30.94	
Error	9	0.08	0.0089		
Total	15	1.29			

8.9 Residual Analysis

Consider a two-way model: $y_{ij} = \mu + \tau_j + \beta_i + \epsilon_{ij}, i = 1, 2, ..., r; j = 1, 2, ..., p$. The assumptions of the model are: $\epsilon_{ij} \sim N(0, \sigma^2)$, and $\sum_{j=1}^{p} \tau_j = 0 = \sum_{i=1}^{r} \beta_i$. The predicted values are $\hat{y}_{ij} = \bar{y}_{i\cdot} + \bar{y}_{\cdot j} - \bar{y}$. Note that $E(y_{ij}) = \mu + \tau_j + \beta_i = (\mu + \tau_j) + (\mu + \beta_i) - \mu = E(\hat{y}_{ij}) = (\hat{\mu} + \hat{\tau}_j) + (\hat{\mu} + \hat{\beta}_i) - \hat{\mu} = \bar{y}_{\cdot j} + \bar{y}_{i\cdot} - \bar{y}$. The residuals can be estimated with $\hat{\epsilon}_{ij} = Y_{ij} - \hat{y}_{ij}$. Using these $\hat{\epsilon}_{ij}$, a test for normality can be performed.

8.10 Latin Square Design

In the randomized block design, we control one source of variability by grouping the experimental units into blocks of homogeneous units. Differences among blocks is removed from the experimental error. To control two or more sources of variation, we need different designs. One such design which controls two sources of variation is the Latin Square design. To construct a Latin Square design for p treatments, we need p^2 experimental units. These p^2 units are first classified into p groups of p units, each based on one source of variability. This is called *row classification.* The units are then classified into p groups of p units each, based on the other source of variation. This is called *column classification.* Treatments are assigned such that each treatment occurs once and only once in each row and column.

Example: There are 3 treatments and 9 experimental units.

	1	2	3
1	A	B	C
2	B	C	A
3	C	A	B

The data can be organized into the following general format:

	Columns				
Rows	1	2	3	...	p
	2			...	p
	3			...	p
	.			...	p
	.			...	p
	.			...	p
	p			...	p

$y_{ij(k)}$ is the yield in the i-th row, j-th column when the k-th treatment is used.

Example: There are five formulations of an explosive mixture. Material is coming from five sources. Preparation is done by different operators. We want to control the variability due to the operators. The five treatments are A, B, C, D, E. Use a Latin square design.

			Operators		
Operators					
	A(24)	B(20)	C(19)	D(24)	E(24)
	B(17)	C(24)	D(30)	E(27)	A(36)
	C(18)	D(38)	E(26)	A(27)	B(21)
	D(26)	E(31)	A(26)	B(23)	C(22)
	E(22)	A(30)	B(20)	C(29)	D(31)

Rows	Columns					Row Means
	1	2	3	...	p	
1						$\bar{R}_1$
2						$\bar{R}_2$
3						$\bar{R}_3$
.						.
.						.
.						.
.						.
p						$\bar{R}_p$
	$\bar{c}_1$	$\bar{c}_2$	$\bar{c}_3$	...	$\bar{c}_p$	

Let $\bar{y}$ be the mean of all the observations. The treatment means are $\bar{T}_1$, $\bar{T}_2$, ..., $\bar{T}_p$. The decomposition of the total sums of squares is $SS(TOTAL) = p\sum_{i=1}^{p}(\bar{R}_i - \bar{y})^2 + p\sum_{i=1}^{p}(\bar{c}_i - \bar{y})^2 + p\sum_{i=1}^{p}(\bar{T}_i - \bar{y})^2 + SS(E) = SS(Rows) + SS(Columns) + SS(TRT) + SS(E)$. SS(E) is deduced by subtracting the other sums from the total sums of squares. The ANOVA table is as follow:

Source	d.f.	SS	MS	F
Rows	$p-1$	SS(Rows)	$\frac{MS(Rows)}{p-1}$	$\frac{MS(Rows)}{MS(E)}$
Columns	$p-1$	SS(Columns)	$\frac{SS(Columns)}{p-1}$	$\frac{MS(Columns)}{MS(E)}$
Treatments	$p-1$	SS(TRT)	$\frac{SS(TRT)}{p-1}$	$\frac{MS(TRT)}{MS(E)}$
Error	$(p-1)(p-2)$	SS(E)	$\frac{SS(E)}{(p-1)(p-2)}$	
Total	p^2-1	SS(Total)		

Test $H_0 : \tau_1 = \tau_2 = \cdots = \tau_p$. $H_1 : \tau_i \neq \tau_j, i, j \in 1, 2, ..., p$. Under $H_0 : F_3 = \frac{MS(TRT)}{MS(E)} \sim F(p-1, (p-1)(p-2))$. To check whether the blocking was effective, row wise and columnwise, by $F_1 > 1 \Rightarrow$ Row variation effective. $F_2 > 1 \Rightarrow$ Column variation effective. The SAS source code for the Latin square design is as follow:

```
DATA A;
INPUT ROW $ COL $ TRT $ Y;
CARDS;
1 1 A 24
1 2 B 20
1 3 C 19
...
;
RUN;

PROC ANOVA;
CLASSES ROW COL TRT;
MODEL Y=ROW COL TRT;
RUN;
```

Source	d.f.	SS	F	p-value
Row	4	68	1.59	
Column	4	150	3.52	
Treatment	4	330	7.73	0.0025
Error	12	128		
Total	24			

8.11 Summary

- *treatment*- a procedure or a set of circumstances that is used in the experiment to study the effect of it on the yield.
- *factor*- a set of similar treatments.
- *levels*- of a factor are the treatments within that factor.

One factor designs:

1. CRD.
2. RBD.
3. LSD.
4. CRD with nesting. Variation in experimental error is broken into sampling error and the expected error variation.
5. CRD 2-stage nesting design. 1 factor, p treatments, and r observations.

8.12 Factorial Designs

In factorial designs, more than one factor is considered. Suppose that there are two factors: A and B. Suppose that factor A has 2 levels, A_1 and A_2. Factor B has 2 levels, B_1 and B_2. The number of treatments is equal to $2(2) = 4$. They are two levels of the first factor plus two levels of the second factor: A1B1, A1B2, A2B1, A2B2. The *effect* of a factor is a change in the measured response caused by a change in the level of that factor. The three effects of interest in a factorial experiment are:

1. Simple effects.
2. Main effects.
3. Interaction effects.

	Factor B		
Factor A	B1	B2	
A1	μ_{11}	μ_{12}	$\bar{\mu}_{1\cdot}$
A2	μ_{21}	μ_{22}	$\bar{\mu}_{2\cdot}$
	$\bar{\mu}_{\cdot 1}$	$\bar{\mu}_{\cdot 2}$	

$\bar{\mu}_{1\cdot} = \frac{1}{2}(\mu_{11} + \mu_{12})$. The *sample effects* for factor A are: $\mu_{12} - \mu_{11}$, $\mu_{22} - \mu_{21}$. The sample effects for factor B are: $\mu_{21} - \mu_{11}$, $\mu_{22} - \mu_{12}$. The *main effects* of factor A are: $A = \bar{\mu}_{2\cdot} - \bar{\mu}_{1\cdot}$. The main effects of factor B are: $B = \bar{\mu}_{\cdot 2} - \bar{\mu}_{\cdot 1}$. The *interaction effect* (between the two factors): $\mu_{11} + \mu_{22} - \mu_{12} - \mu_{21}$.

When the lines are parallel, there is no interaction between the two factors.

When the lines have different heights, there is interaction between the two factors. If there is any interaction, then the main effects formulas do not have any interaction. Hence, in these problems we test for the absence of interaction.

Example: Measure the effect of two gasoline additives, T and P, alone and in combinations on gas mileages. The 2 factors are T and P. There are 2 levels of each factor: P_0(absence) and P_1(presence), T_0(absence) and

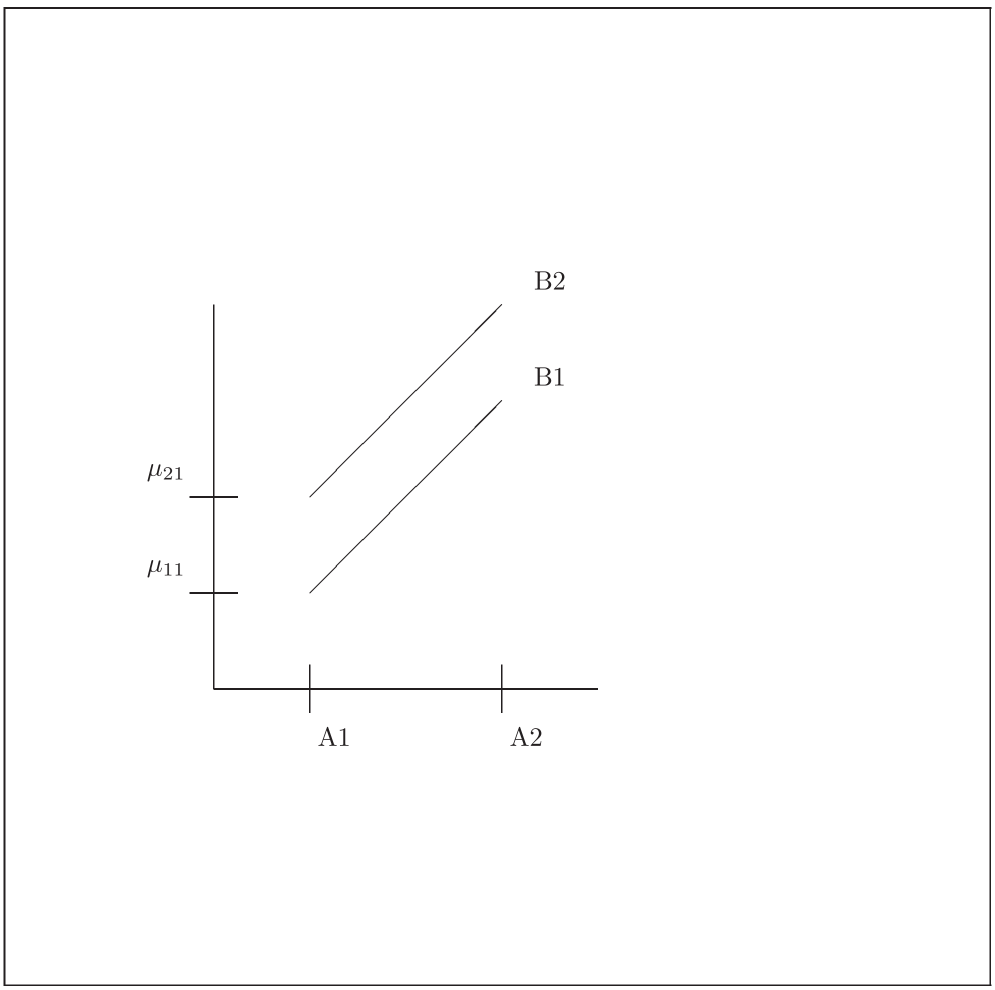

Figure 8.4: Parallel lines indicate no interaction.

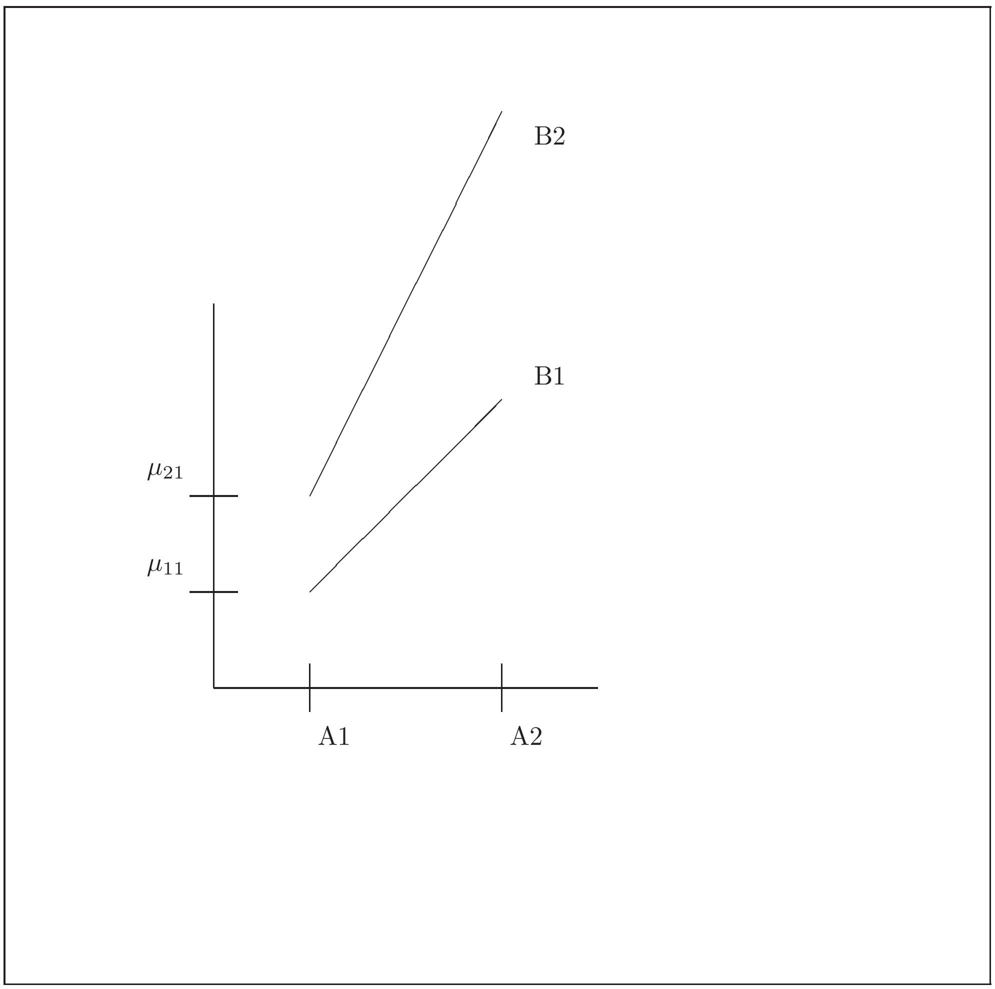

Figure 8.5: Lines with different heights indicate interaction.

T_1(presence). The 4 treatments are T_0P_0, T_1P_0, T_0P_1, and T_1P_1. The mean gas mileages are:

	P_0	P_1	
T_0	20	30	25
T_1	40	52	46
	30	41	

To estimate the interaction effect: $72 - 70 = 2$. To estimate the main effect of: $T = 46 - 25 = 21$. $P = 41 - 30 = 11$.

8.12.1 2-Factor Factorial Design

By factorial design, we mean that in each complete trial or replication, all possible combinations of the levels of the factors are investigated.

Example: Suppose there are 2 factors, say A and B. Let factor A have a levels and factor B have b levels. Arranging this in a factorial design would mean $a(b)$ treatments are investigated in each replication. In general, we can have r replications. In this case, we would need rab experimental units for this factorial design.

Example: An engineer is designing a battery for use in a device that will be subjected to extreme variations in temperatures. The design parameters that can be controlled are the plate material: Plate 1, Plate 2, and Plate 3. In a controlled lab experiment, 3 temperatures are used to represent variations of temperature. We have 2 factors: 1) Material(with 3 levels) and 2) Temperature(with 3 levels). Denote the material levels by μ_1, μ_2, μ_3 and the temperature levels by T_1, T_2, T_3. There are $a(b) = 3(3) = 9$ treatments. There were four replications of the experiment. In all 4(9) experimental runs were made. Randomization: Randomly select 4 units and use treatment $1(\mu_1 T_0)$. Randomly select another 4 units and used $\mu_2 T_1$ as in a completely randomized design. Continue until there are no more experimental runs.

Data:

	T_1	T_2	T_3
μ_1	155, 130, 74, 180	34, 40, 80, 75	20, 70, 82, 78
μ_2	150, 185, 159, 126	136, 122, 106, 115	25, 70, 58, 45
μ_3	138, 110, 168, 160	174, 120, 150, 136	96, 104, 82, 60

Analysis of the data: The decomposition of the sums of squares is as follow: $SS(TOT) = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{r}(y_{ijk} - \bar{y})^2$, where $\bar{y} = \frac{1}{abr}\sum\sum\sum y_{ijk}$. Then,

$$\overbrace{rb\sum_{i=1}^{a}(\bar{y}_{i\cdot\cdot} - \bar{y})^2}^{\text{SS(A)}} + \overbrace{ra\sum_{j=1}^{b}(\bar{y}_{\cdot j\cdot} - \bar{y})^2}^{\text{SS(B)}} + \overbrace{r\sum_{i=1}^{a}\sum_{j=1}^{b}(\bar{y}_{ij\cdot} - \bar{y}_{i\cdot\cdot} - \bar{y}_{\cdot j\cdot} + \bar{y})^2}^{\text{SS(AB)}} + \overbrace{\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{r}(y_{ijk} - \bar{y}_{ij\cdot})^2}^{\text{SS(E)}}.$$

Model: $y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \epsilon_{ijk}, k = 1, 2, ..., r; j = 1, 2, ..., b; i = 1, 2, ..., a$. μ is the overall mean. α_i is the effect of the i-th level of factor A. β_j is the effect of the j-th level of factor B. $(\alpha\beta)_{ij}$ is the interaction of the i-th level of factor A with the j-th level of factor B. ϵ_{ijk} is the random experimental error and is $N(0, \sigma^2)$.

Hypotheses of interest:

1. $H_{01} : \alpha_1 = \alpha_2 = ... = \alpha_a$. No main effect of factor A.
2. $H_{02} : \beta_1 = \beta_2 = ... = \beta_b$. No main effect of factor B.
3. $H_{03} : (\alpha\beta)_{ij} = \gamma, \forall ij$. There is no interaction between factor A and factor B.

The ANOVA table:

Source	d.f.	SS	MS	E(MS)
Factor A	$a-1$	SS(A)	$\frac{SS(A)}{a-1}$	$\sigma^2 + \theta_A^2$
Factor B	$b-1$	SS(B)	$\frac{SS(B)}{b-1}$	$\sigma^2 + \theta_B^2$
Interaction AB	$(a-1)(b-1)$	SS(AB)	$\frac{SS(AB)}{(a-1)(b-1)}$	$\sigma^2 + \theta_{AB}^2$
Error	$ab(r-1)$	SS(E)	$\frac{SS(E)}{ab(r-1)}$	σ^2
Total	$abr-1$	SS(TOT)		

$\theta_A^2 = \frac{1}{a-1}\sum_{i=1}^a(\alpha_i - \bar{\alpha})^2$. $\theta_B^2 = \frac{1}{b-1}\sum_{j=1}^b(\beta_j - \bar{\beta})^2$. $\theta_{AB}^2 = \frac{1}{(a-1)(b-1)}\sum_{i=1}^a\sum_{j=1}^b\left[(\alpha\beta)_{ij} - (\bar{\alpha}\bar{\beta})_{i\cdot} - (\bar{\alpha}\bar{\beta})_{\cdot j} + (\bar{\alpha}\bar{\beta})\right]^2$. The F statistics are: $F_A = \frac{MS(A)}{MS(E)} \sim F(a-1, ab(r-1))$. $F_B = \frac{MS(B)}{MS(E)} \sim F(b-1, ab(r-1))$. $F_{AB} = \frac{MS(AB)}{MS(E)} \sim F[(a-1)(b-1), ab(r-1)]$. Note that in practice, always test H_{03}(no interaction) first. If H_{03} is rejected, H_{02} and H_{01} will not have the same meaning as noted.

For the data in the example,

Source	d.f.	SS	MS	F
A	2	10683.72	5341.86	7.91
B	2	39118.72	19559.36	28.97
AB	4	9613.78	2403.445	3.56
Error	27	18230.75	675.213	
Total	35	77646.97		

Since $3.56 > 2.73$, there is an interaction between factor A and factor B. Now, consider all 9 treatments and do multiple comparisons to identify the best treatments.

Means table:

	T_1	T_2	T_3
M_1	134.75	57.25	57.25
M_2	155.75	119.75	49.5
M_3	144.00	145.75	85.5

8.13 2-Factor, Crossed Designs

Factor A has a levels. Factor B has b levels. The design will produce ab treatments per run. With replication, we will need rab experimental units.

The model statement is $y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \epsilon_{ijk}, i = 1, 2, ..., a; j = 1, 2, 3, ..., b; k = 1, 2, ..., r$.

Case 1: If the interaction hypothesis is rejected, perform multiple comparisons to test the interaction data only. Multiple comparisons of the interactions will yield the best choice of i and j. $E(y_{ijk}) = \mu_{ij}$ is the mean of the i-th level of factor A and the j-th level of factor B. The least square estimate of μ_{ij} is $\hat{\mu} = \bar{y}_{ij\cdot} = \frac{1}{r}\sum_{k=1}^{r} y_{ijk}$. The standard error of $\hat{\mu}_{ij} = \sqrt{\frac{MS(E)}{r}}$. A $100(1-\alpha)\%$ confidence interval for μ_{ij} is $\bar{y}_{ij\cdot} \pm t_{\alpha/2}(ab(r-1))\sqrt{\frac{MS(E)}{r}}$. The confidence interval for a contrast, $\mu_{12} - \mu_{13} = (\bar{y}_{12\cdot} - \bar{y}_{13\cdot}) \pm t_{\alpha/2}(ab(r-1))\sqrt{\frac{MS(E)}{r}}$.

Case 2: No interaction effect. If $(\alpha\beta)_{ij} = 0$ is accepted, we will compute the main effect results.

1. Suppose $H_0 : \alpha_1 = \alpha_2 = \cdots = \alpha_a$ is rejected. Perform an analysis of the means for factor A. $\mu_{i\cdot} = \mu + \alpha_i$ is the mean of the i-th level of factor A. Estimate $\mu_{i\cdot} = \hat{\mu}_{i\cdot} = \frac{1}{br}\sum_{j=1}^{b}\sum_{k=1}^{r} y_{ijk}$. The standard error is given by $\sqrt{\frac{MS(E)}{br}}$.
2. Suppose $H_0 : \beta_1 = \beta_2 = \cdots = \beta_b$ is rejected. Estimate $\mu_{\cdot j} = \mu + \beta_j = \hat{\mu}_{\cdot j} = \bar{y}_{\cdot j\cdot} = \sum_{i=1}^{a}\sum_{k=1}^{r} y_{ijk}$. The standard error is given by $\sqrt{\frac{MS(E)}{ar}}$.

8.13.1 2-Factor Factorial Design with r Blocks

There are ab treatments applied to each block. Model: $y_{ijk} = \mu + B_k + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \epsilon_{ijk}, i = 1, 2, ..., a; j = 1, 2, ..., b; k = 1, 2, ..., r$. μ is the overall mean. B_k is the effect of the k-th block. α_i is the effect of the i-th level of factor A. β_j is the effect of the j-th level of factor B. $(\alpha\beta)_{ij}$ is the effect of the interaction. The ANOVA table for a blocked 2-factor factorial design:

Source	d.f.	SS	MS	F
Block	$r-1$	SS(BLOCK)	MS(BLOCK)	$\frac{MS(BLOCK)}{MS(E)} \Rightarrow F_1$
A	$a-1$	SS(A)	MS(A)	$\frac{MS(A)}{MS(E)} \Rightarrow F_2$
B	$b-1$	SS(B)	MS(B)	$\frac{MS(B)}{MS(E)} \Rightarrow F_3$
AB	$(a-1)(b-1)$	SS(AB)	MS(AB)	$\frac{MS(AB)}{MS(E)} \Rightarrow F_4$
Error	$(r-1)(ab-1)$	SS(E)	MS(E)	
Total	$abr-1$	SS(TOTAL)		

Note that if the interaction is significant, do not evaluate the main effects.

8.13.2 2-Factor Random Effects Design

Model: $y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \epsilon_{ijk}, i = 1, 2, ..., a; j = 1, 2, ..., b; k = 1, 2, ..., r$.

Assumptions:

1. $\alpha_i \sim N(0, \theta_\alpha^2)$.
2. $\beta_j \sim N(0, \theta_\beta^2)$.
3. $(\alpha\beta)_{ij} \sim N(0, \theta_{(\alpha\beta)}^2)$.
4. $\epsilon_{ijk} \sim N(0, \theta^2)$.

The ANOVA table for the 2-factor random effects design:

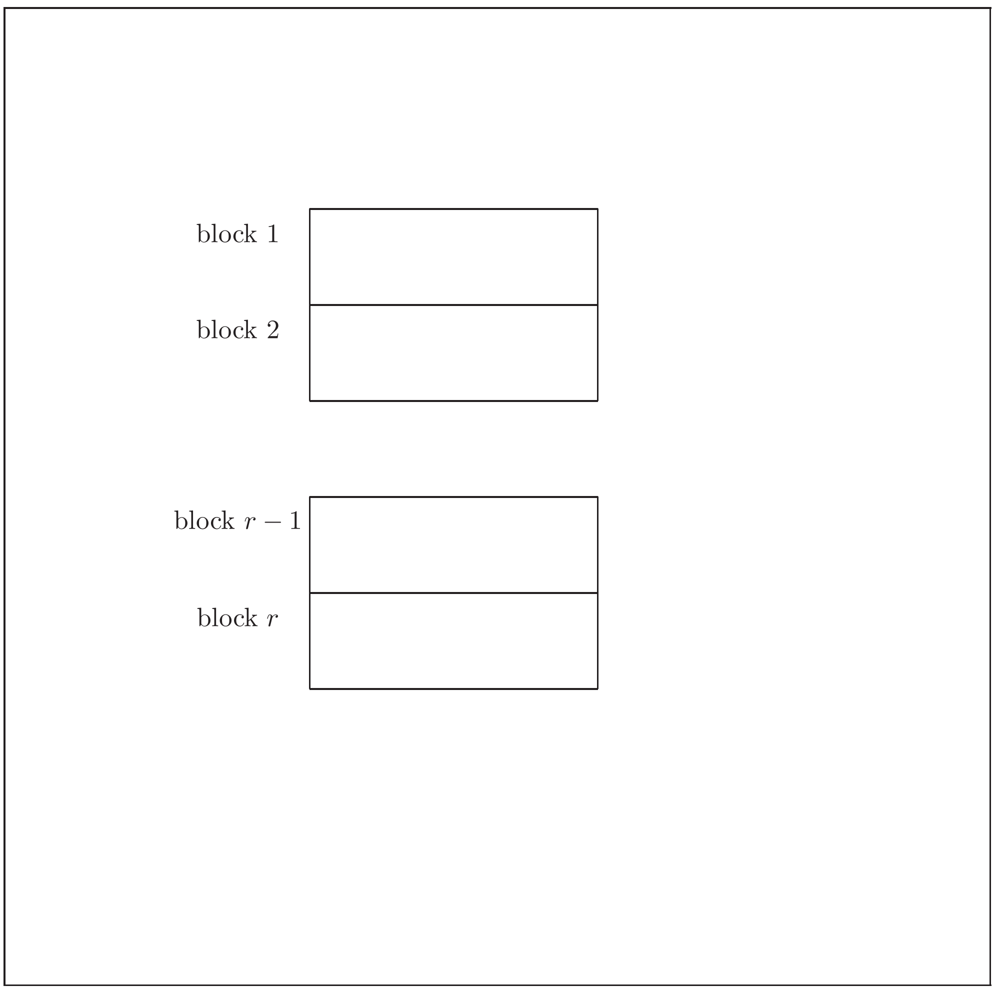

Figure 8.6:

Source	d.f.	MS	E(MS)
A	$a-1$	MS(A)	$\theta^2 + r\theta^2_{(\alpha\beta)} + ar\theta^2_\beta + br\theta^2_\alpha$
B	$b-1$	MS(B)	$\theta^2 + r\theta^2_{(\alpha\beta)} + ar\theta^2_\beta$
AB	$(a-1)(b-1)$	MS(AB)	$\theta^2 + r\theta^2_{(\alpha\beta)}$
Error	$ab(r-1)$	MS(E)	θ^2
Total	$abr-1$		

If no interaction, $r\theta^2_{(\alpha\beta)} = 0 \Rightarrow F_3$, then evaluate F_1 and F_2. PROC VARCOM in SAS will give the % variance components. Estimation of the variance components is as follow: $\theta^2_{(\alpha\beta)} = \frac{MS(AB)-MS(E)}{r}$.

8.13.3 2-Factor Mixed Effects Design

Factor A is fixed in this model. The model statement is the same as before. The ANOVA table is:

Source	d.f.	MS	E(MS)
A(fixed)	$a-1$	MS(A)	$\theta^2 + r\theta^2_{(\alpha\beta)} \frac{br}{a-1} \sum_{i=1}^{a} (\alpha_i - \bar{\alpha})^2$
B(random)	$b-1$	MS(B)	$\theta^2 + r\theta^2_{(\alpha\beta)} + ar\theta^2_\beta$
AB	$(a-1)(b-1)$	MS(AB)	$\theta^2 + r\theta^2_{(\alpha\beta)}$
Error	$ab(r-1)$	MS(E)	θ^2
Total	$abr-1$		

8.14 3-Way Factorial Design

There are three factors A, B, C. There are a levels of factor A, b levels of factor B, and c levels of factor C. In all there are abc treatments. We need $rabc$ experimental units to have r replications of the experiment. Let y_{ijkl} be the observation on the i-th level of factor A, the j-th level of factor B, the k-th level of factor C and in the l-th replication. Model: $y_{ijkl} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \gamma_k + (\alpha\gamma)_{ik} + (\beta\gamma)_{jk} + (\alpha\beta\gamma)_{ijk} + \epsilon_{ijkl}, i = 1, 2, ..., a; j = 1, 2, ..., b; k = 1, 2, ..., c; l = 1, 2, ..., r$. Assume that $\epsilon_{ijkl} \sim N(0, \sigma^2)$.

Source	d.f.	SS	MS	F
A	$a-1$	SS(A)	$\frac{SS(A)}{a-1}$	$\frac{MS(A)}{MS(E)}$
B	$b-1$	SS(B)	$\frac{SS(B)}{b-1}$	$\frac{MS(B)}{MS(E)}$
AB	$(a-1)(b-1)$	SS(AB)	$\frac{SS(AB)}{(a-1)(b-1)}$	$\frac{MS(AB)}{MS(E)}$
C	$c-1$	SS(C)	$\frac{SS(C)}{c-1}$	$\frac{MS(C)}{MS(E)}$
AC	$(a-1)(c-1)$	SS(AC)	$\frac{SS(AC)}{(a-1)(c-1)}$	$\frac{MS(AC)}{MS(E)}$
BC	$(b-1)(c-1)$	SS(BC)	$\frac{SS(BC)}{(b-1)(c-1)}$	$\frac{MS(BC)}{MS(E)}$
ABC	$(a-1)(b-1)(c-1)$	SS(ABC)	$\frac{SS(ABC)}{(a-1)(b-1)(c-1)}$	$\frac{MS(ABC)}{MS(E)}$
Error	$(r-1)(abc-1)$	SS(E)	$\frac{SS(E)}{(r-1)(abc-1)}$	
Total	$rabc-1$	SS(TOTAL)		

The sums of squares are derived similarly to those in the 2-factored designs. The hypotheses are as follow:

	H_0
A	$\sum_{i=1}^{a} \alpha_i = 0$
B	$\sum_{j=1}^{b} \beta_j = 0$
AB	$\sum_{i=1}^{a} \sum_{j=1}^{b} (\alpha\beta)_{ij} = 0$
C	$\sum_{k=1}^{c} \gamma = 0$
AC	$\sum_{i=1}^{a} \sum_{k=1}^{c} (\alpha\gamma)_{ik} = 0$
BC	$\sum_{j=1}^{b} \sum_{k=1}^{c} (\beta\gamma)_{jk} = 0$
ABC	$\sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{k=1}^{c} (\alpha\beta\gamma)_{ijk} = 0$

Example: (last class, these notes seem to be missing). There are 3 factors: 1) pressure with 2 levels: 25psi and 30psi, 2) Speed with 2 levels: 200rmp and 250rmp, and 3) % carbonation with 3 levels: 10%, 12%, and 14%. The number of treatments is $(2)(2)(3) = 12$. The number of replications is 2. The SAS source code is as follow:

```
DATA A;
INPUT PRESSURE $ SPEED $ CARBO $ Y;
CARDS;
25 200 10 -3
25 200 10 -1
...
30 250 14 11
;
RUN;

PROC ANOVA;
CLASS PRESSURE SPEED CARBO;
MODEL Y=PRESSURE|SPEED|CARBO;
RUN;
```

Source	d.f.	SS	MS	F	p
Pressure	1	45.375	45.375	64.06	0.0001
Speed	1	22.442	22.442	31.12	0.0001
Press. & Speed	1	1.042	1.042	1.47	0.2486
Carbonation	2	252.75	126.375	178.41	0.0001
Press. & Carb.	2	5.25	2.625	3.71	0.0558
Speed & Carb.	2	0.583	0.2915	0.41	0.675
Press. & Speed & Carb.	2	1.083	0.5415	0.76	0.487
Error	12	8.50	0.708		
Total	23	336.625			

Conclusions: No interaction among all three factors. Speed/Carbonation and Pressure/Speed are significant at $\alpha = 0.10$. There is interaction between pressure and carbonation. The main factor speed is significant. The different levels of speed produce different results. The means for speed are:

200	250
2.167	4.08

Recommed speed set to 200rpm. Next, pressure and carbonation:

	25psi	30psi
10%	-1.25	0.25
12%	1	4
14%	5.5	9.25

Recommed 10% carbonation and pressure at 300psi.

8.15 Homework and Answers

0. For the mixed and random effects models, estimate all the variance components. $E(MSE) = \sigma^2 \Rightarrow \hat{\sigma}^2 = MSE$. $E(MS(N)) = \sigma^2 + n\sigma^2_\beta \Rightarrow \hat{\sigma}^2 + n\hat{\sigma}^2_\beta = MS(N)$. Thus, $\hat{\sigma}^2_\beta = \frac{MS(N)-MS(E)}{n}$.

1. A genetics study with beef animals consisted of several sires each mated to a separate group of dams. The matings that resulted in male progeny calves were used for an inheritance study of birth weights. The birth weights of eight male calves in each of five sire groups are

Sire	Birthweights								$\bar{Y}_{i\cdot}$
1	61	100	56	113	99	103	75	62	83.625
2	75	102	95	103	98	115	98	94	97.500
3	58	60	60	57	57	59	54	100	63.125
4	57	56	67	59	58	121	101	101	77.500
5	59	46	120	115	115	93	105	75	91.000

Assuming a random effects model analyze the data. Estimate the interclass correlation coefficient. Intraclass correlation measure the similarity of observations within a treatment(or group). Interpret the correlation you have obtained. In this experiment, the sires are the treatments. The experimental units are calves. The number of replications is equal per treatment. Thus, $p = 5$, and $r = 8$. In the random effects model, the following equation is used, $y_{ij} = \mu + \tau_i + \epsilon_{ij}, i \in 1, ..., 5, j \in 1, ..., 8$. y_{ij} is the j-th observation on the i-th treatment. μ is the overall mean of all the observations. τ_i is a random effect associated with the i-th treatment. ϵ_{ij} is the random error associated with the j-th observation on the i-th treatment. The assumptions for this model are as follow:

1. Each population has the same variance, and

   $$\tau_i \sim N(0, \sigma^2_\tau)$$

2. The random effects are normally distributed.

   $$\epsilon_{ij} \sim N(0, \sigma^2)$$

The ANOVA Table that will be used in this experiment is as follows:

ANOVA Table Format

Source	d.f.	SS	MS	E(MS)
Trt	$p-1$	$r\sum_{i=1}^{p}(y_{i\cdot} - \bar{y})^2$	$\frac{SST}{p-1}$	$\sigma^2 + r\sigma^2_\tau$
Error	$p(r-1)$	$\sum_{i=1}^{p}\sum_{j=1}^{r}(y_{i,j} - \bar{y}_{i\cdot})^2$	$\frac{SSE}{p(r-1)}$	σ^2
Total	$rp-1$	$SST + SSE$		

Filling in the table using the SAS printout yields,

ANOVA Table of Sires

Source	d.f.	SS	MS	E(MS)	F	p-value
Treatment	4	5591.15	1397.7875	1397.7875	3.01	0.0309
Error	35	16232.75	463.7928571	463.7928571		
Total	39	21823.90				

To estimate σ_τ^2, the following equation is used: $\hat{\sigma}_\tau^2 = \frac{MST-MSE}{r}$. So, substituting in values from the ANOVA Table yields, $\hat{\sigma}_\tau^2 = \frac{1397.7875-463.7928571}{8} = 116.7493304$. The following hypothesis test is used: $H_0 : \sigma_\tau^2 = 0$ versus $H_a : \sigma_\tau^2 > 0$ The F statistic is used to test the hypothesis. The theoretical value of F at $\alpha = 0.05$ level is approximately 2.69. Since $3.01 > 2.69$, the null hypothesis is rejected. There is a significance difference among the means. The intraclass correlation coefficient is estimated as follow: $p = \frac{\sigma_\tau^2}{\sigma^2+\sigma_\tau^2} = \frac{116.7493304}{463.7928571+116.7493304} = 0.201$.

2. A soil scientist studied the growth of barley plants under three different levels of salinity in a controlled growth medium. There were two replicate containers for each treatment in a completely randomized design and three plants were measured in each replication. The data on dry weight of plants in grams are

Salinity	Container	Weight (g)			$\bar{Y}_{ij\cdot}$	$\bar{Y}_{i\cdot\cdot}$
Control	1	11.29	11.08	11.10	11.157	9.315
	2	7.37	6.55	8.50	7.473	
6 bars	3	5.64	5.98	5.69	5.77	4.8435
	4	4.20	3.34	4.21	3.917	
12 bars	5	4.83	4.77	5.66	5.087	3.9735
	6	3.28	2.61	2.69	2.86	

Analyze these data by writing an appropriate model. A mixed effects nested model will be used to model the data. The treatments are the different levels of salinity. There are 3 treatments. The nesting factor is the different containers. There are 6 containers — two per treatment. In a mixed effects model the following equation is used: $Y_{ijk} = \mu_i + \beta_{ij} + \epsilon_{ijk}$ μ_i is the effect of the i-th level of the treatment and is fixed. β_{ij} is the effect of the j-th level of the nested factor in the i-th level of the treatment and is random. ϵ_{ijk} is the error of each sample and is random. The assumptions for this model are as follow:

1. $\beta_{ij} \sim N(0, \sigma_\beta^2)$.
2. $\epsilon_{ijk} \sim N(0, \sigma^2)$.

The ANOVA Table format is as follow:

ANOVA Table Format

Source	d.f.	SS	MS	E(MS)
Treatment	$p-1$	$nr\sum_{i=1}^{p}(y_{i\cdot\cdot} - \bar{y})^2$	$\frac{SST}{p-1}$	
Nesting	$p(r-1)$	$n\sum_{i=1}^{p}\sum_{j=1}^{r}(\bar{y}_{ij\cdot} - \bar{y}_{i\cdot})^2$	$\frac{SSN}{p(r-1)}$	$E(MSN)$
Error	$rp(n-1)$	$\sum_{i=1}^{p}\sum_{j=1}^{r}\sum_{k=1}^{n}(y_{ijk} - \bar{y}_{ij\cdot})^2$	$\frac{SSE}{pr(n-1)}$	$E(MSE)$
Total	$npr-1$	$SST + SSN + SSE$		

The expected values are estimated as follow:

- $E(MST) = \sigma^2 + n\sigma_\beta^2 + \frac{rn}{p-1}\sum_{i=1}^{p}(\mu_i - \bar{\mu})^2 = 60.538087$.
- $E(MSN) = \sigma^2 + n\sigma_\beta^2 = 11.25525256$.

– $E(MSE) = \sigma^2 = 0.27275556$.

Filling in the table using the SAS printout yields,

ANOVA Table of Salinity

Source	d.f.	SS	MS	E(MS)	F
Treatment	2	2.448	1.224		4.488
Nesting	3	32.93975	10.97991667		40.26
Error	12	3.27306667	0.27275556		
Total	17	134.78502778			

The confidence intervals at $\alpha = 0.05$ level of significance are given by the following equation: $\bar{Y}_i = t_{0.025}(12)\sqrt{\frac{MSE}{n}}, i = 1, ..., 3$. So, $\bar{Y}_i = 2.179\sqrt{\frac{.27275556}{6}} = 0.4646, i = 1, ..., 3$. Substituting in the actual means yields,

– For the Control: [8.850, 9.780].

– For 6 bars: [4.379, 5.308].

– For 12 bars: [3.509, 4.438].

To test the F_2 statistic, the following hypothesis is used: $H_0 : \beta_{i,1} = \beta_{i,2}, i = 1, ..., 3$ versus $H_a : \beta_{i,1} \neq \beta_{i,2}, i = 1, ..., 3$. The theoretical value for F_2 is $F_{p(r-1),rp(n-1)} = F_{(3,12)} = 3.77$ at $\alpha = 0.05$. Since $40.26 > 3.77$ the null hypothesis is rejected. The nesting factor is effective. The second hypothesis is as follow: $H_0 : \mu_1 = \mu_2 = \mu_3$ versus $H_a : \mu_i \neq \mu_j, i \neq j, i, j \in 1, ..., 3$. The theoretical value for F_1 is $F_{(p-1),p(r-1)} = F_{(2,3)} = 4.50$ at $\alpha = 0.05$. Since $4.488 < 4.50$, the means are the same.

3. Consider a company that purchases its raw material from three different suppliers. The company wishes to determine if the purity of the raw material is the same from each supplier. Each supplier supplies the material in four batches. Three determinations of purity are taken in the experiment from each batch. The data in a coded form are

Suppliers

	1				2				3			
	1	2	3	4	1	2	3	4	1	2	3	4
	1	-2	-2	1	1	0	-1	0	2	-2	1	3
	-1	-3	0	4	-2	4	0	3	4	0	-1	2
	0	4	1	0	-3	2	-2	2	0	2	2	1
$Y_{ij.}$	0.00	-0.333	-0.333	1.667	-1.333	2.00	-1.00	1.667	2.00	0.00	0.667	2.00
$\bar{Y}_{i..}$	0.25				0.333				1.167			

Analyze these data to address company's wish. A fixed effects nested model will be used to model the data. There are 3 suppliers that make-up the main factor and 4 batches per supplier(the nested factor). The following equation is used to model the data: $Y_{ijk} = \mu_i + \beta_{ij} + \epsilon_{ijk}$ μ_i is the effect of the i-th level of the treatment and is fixed. β_{ij} is the effect of the j-th level of the nested factor in the i-th level of the treatment and is fixed. ϵ_{ijk} is the error of each sample and is random. The assumption for this model is that $\epsilon_{ijk} \sim N(0, \sigma^2)$. The ANOVA Table format has the following format:

ANOVA Table Format

Source	d.f.	SS	MS	E(MS)
Trt	$p-1$	$np\sum_{i=1}^{p}(y_{i\cdot\cdot}-\bar{y})^2$	$\frac{SST}{p-1}$	$E(MST)$
Nest	$p(r-1)$	$n\sum_{i=1}^{p}\sum_{j=1}^{r}(\bar{y}_{ij\cdot}-\bar{y}_{i\cdot})^2$	$\frac{SSN}{p(r-1)}$	$E(MSN)$
Error	$rp(n-1)$	$\sum_{i=1}^{p}\sum_{j=1}^{r}\sum_{k=1}^{n}(y_{ijk}-\bar{y}_{ij\cdot})^2$	$\frac{SSE}{pr(n-1)}$	$E(MSE)$
Total	$npr-1$	$SST+SSN+SSE$		

The expected values are as follow:

- $E(MST)=\sigma^2+\frac{np}{p-1}\sum_{i=1}^{p}(\mu_i-\bar{\mu})^2=11.01857567.$
- $E(MSN)=\sigma^2+\frac{n}{p(r-1)}\sum_{i=1}^{p}\sum_{j=1}^{r}(\beta_{ij}-\bar{\beta}_i)^2=8.703574667.$
- $E(MSE)=\sigma^2=3.75.$

Filling in the table using the SAS printout yields,

ANOVA Table of Salinity

Source	d.f.	SS	MS	E(MS)	F
Treatment	2	6.1666667	3.083333333	11.01857567	0.82
Nesting	9	44.58333333	4.95370370	8.703574667	1.32
Error	24	90.0000	3.75	3.75	
Total	35	140.75			

The equation for a $\alpha=0.05$ confidence interval is given by the following equation: $\bar{Y}_i=t_{0.025}(24)\sqrt{\frac{MSE}{n}}, i=1,...,3$. So, $\bar{Y}_i=2.064\sqrt{\frac{3.75}{12}}=1.154, i=1,...,3$. Substituting in the actual means yields,

- For Supplier No. 1: [-0.904, 1.404].
- For Supplier No. 2: [-0.821, 1.487].
- For Supplier No. 3: [0.013, 2.321].

To test the F_2 statistic, the following hypothesis is used: $H_0:\beta_{i,1}=\beta_{i,2}=\beta_{i,3}=\beta_{i,4}, i=1,...,3$ versus $H_a:\beta_{i,j}\neq\beta_{i,k}, i=1,...,3, j,k\in 1,...,4$. The theoretical value for F_2 is $F_{p(r-1),rp(n-1)}=F_{(9,24)}=4.81$ at $\alpha=0.05$. Since $1.32<4.81$ the null hypothesis is accepted. The nesting factor is not effective. The second hypothesis is as follow: $H_0:\mu_1=\mu_2=\mu_3$ versus $H_a:\mu_i\neq\mu_j, i\neq j, i,j\in 1,...,3$. The theoretical value for F_1 is $F_{(p-1),p(r-1)}=F_{(2,9)}=3.20$ at $\alpha=0.05$. Since $0.82<3.20$, the means are the same.

8.16 Homework and Answers

1. A fertilizer trial on a range grass, blue grama, was conducted in a randomized complete block design. Five fertilizer treatments were randomly assigned to the plots in each of five blocks. The data are percent phosphorus in a plant tissue sample from each plot.

	BLOCK					
Treatment	1	2	3	4	5	
No fertilizer	7.6	8.1	7.3	7.9	9.4	8.06
50 lb nitrogen(N)	7.3	7.7	7.7	7.7	8.2	7.72
100 lb N	6.9	6.0	5.6	7.4	7.0	6.58
50 lb N + 75 lb P_2O_5	10.8	11.2	9.0	12.9	11.6	11.10
100 lb N + 75 lb P_2O_5	9.6	9.3	12.0	10.6	10.4	10.38
	8.44	8.46	8.32	9.30	9.32	8.768

So that the notation in the book works with this set of data, the data is rearranged into the following format:

Blk	No fltzr	50lb N	100lb N	50lb N+75lb P_2O_2	100lb N+75lb P_2O_2
1	7.6	7.3	6.9	10.8	9.6
2	8.1	7.7	6.0	11.2	9.3
3	7.3	7.7	5.6	9.0	12.0
4	7.9	7.7	7.4	12.9	10.6
5	9.4	8.2	7.0	11.6	10.4
	8.06	7.72	6.58	11.10	10.38

a. Write a linear model for this experiment, explain the terms, and compute the analysis of variance to perform the usual tests. The model statement is as follow: $Y_{ij} = \mu + \tau_j + \beta_i + \epsilon_{ij}, i = 1, ..., 5, j = 1, ..., 5$.

- $*$ Y_{ij} is the observation of the $j-th$ treatment on the $i-th$ block.
- $*$ μ is the overall mean.
- $*$ τ_j is the effect of the $j-th$ treatment.
- $*$ β_i is the effect of the $i-th$ block.
- $*$ ϵ_{ij} is the error on the $j-th$ treatment in the $i-th$ block.

The assumptions of the model are as follow:

1. $\epsilon_{ij} \sim N(0, \sigma^2)$.
2. $\beta_i \sim N(, \sigma^2_\beta)$.

The ANOVA Table is as follow:

Source	d.f.	SS
Treatment	$p-1$	$r\sum_{j=1}^{p}(\bar{Y}_{\cdot j} - \bar{Y})^2$
Blocking	$r-1$	$p\sum_{i=1}^{r}(\bar{Y}_{i\cdot} - \bar{Y})^2$
Error	$(r-1)(p-1)$	$\sum_{i=1}^{r}\sum_{j=1}^{p}(Y_{ij} - \bar{Y}_{i\cdot} - \bar{Y}_{\cdot j} + \bar{Y})^2$
Total	$pr-1$	$\sum_{i=1}^{r}\sum_{j=1}^{p}(Y_{ij} - \bar{Y})^2$

The F values are estimated as follow: $F_1 = MS(T)/MS(E)$. $F_2 = MS(B)/MS(E)$. Substituting in the data into the ANOVA Table yields,

Source	d.f.	SS	MS	F	$p-$value
Treatment	4	72.1184	18.0296	22.6048	0.0001
Blocking	4	4.9544	1.2386	1.5529	0.2347
Error	16	12.7616	0.7976		
Total	24	89.8344			

The confidence intervals for the treatments are as follow:

- $*$ No Fertilizer: $\bar{Y} \pm t_{0.025}(16)\sqrt{\frac{MSE}{r}} = 8.06 \pm \frac{2.120\sqrt{0.7976}}{\sqrt{5}} = [7.213, 8.907]$.
- $*$ 50 lb nitrogen(N): $\bar{Y} \pm t_{0.025}(16)\sqrt{\frac{MSE}{r}} = 7.72 \pm \frac{2.120\sqrt{0.7976}}{\sqrt{5}} = [6.873, 8.567]$.
- $*$ 100 lb N: $\bar{Y} \pm t_{0.025}(16)\sqrt{\frac{MSE}{r}} = 6.58 \pm \frac{2.120\sqrt{0.7976}}{\sqrt{5}} = [5.733, 7.427]$.

- 50 lb N + 75 lb P_2O_5 : $\bar{Y} \pm t_{0.025}(16)\sqrt{\frac{MSE}{r}} = 11.10 \pm \frac{2.120\sqrt{0.7976}}{\sqrt{5}} = [10.253, 11.947]$.
- 100 lb N + 75 lb P_2O_5 : $\bar{Y} \pm t_{0.025}(16)\sqrt{\frac{MSE}{r}} = 10.38 \pm \frac{2.120\sqrt{0.7976}}{\sqrt{5}} = [9.533, 11.227]$.

The standard error on the difference of two means is given by, $\sqrt{\frac{2MS(E)}{r}} = \sqrt{\frac{2(0.7976)}{5}} = 0.565$. The confidence intervals for two means follows. $(\bar{Y}_{.j} - \bar{Y}_{.j'}) \pm \frac{2.120\sqrt{2(0.7976)}}{\sqrt{5}}$.

b. Was the blocking effective? Estimating the *relative efficiency* will determine whether blocking was effective. The relative efficiency is given by the following equation: $\frac{(r-1)MS(B)+r(p-1)MS(E)}{(rp-1)MS(E)} = \frac{(4)(1.2386)+5(4)(0.7976)}{(24)(0.7976)} = 1.09215 \geq 1$. Blocking was effective. To test that the means are different, evaluate the F_1 statistic. The hypothesis is stated as follow: $H_0 : \tau_1 = \tau_2 = \tau_3 = \tau_4 = \tau_5$ versus $H_1 : \tau_i \neq \tau_j, i, j \in 1, 2, ..., 5$. $F_{0.05}(4, 16) = 3.01$. Since $22.6048 > 3.01$, the treatment means are significantly different. The null hypothesis is rejected.

2. A traffic engineer conducted a study to compare the total unused red light time for five different traffic signal sequences. The experiment was conducted with a Latin square design in which the two blocking factors were (1) five randomly selected intersections and (2) five time periods. In the data table the five signal sequence treatments are shown in parentheses as A, B, C, D, E and the numerical values are the unused red light times in minutes.

	Time Period					
Intersection	1	2	3	4	5	
1	15.2(A)	33.8(B)	13.5(C)	27.4(D)	29.1(E)	23.80
2	16.5(B)	26.5(C)	19.2(D)	25.8(E)	22.7(A)	22.14
3	12.1(C)	31.4(D)	17.0(E)	31.5(A)	30.2(B)	24.44
4	10.7(D)	34.2(E)	19.5(A)	27.2(B)	21.6(C)	22.64
5	14.6(E)	31.7(A)	16.7(B)	26.3(C)	23.8(D)	22.62
	13.82	31.52	17.18	27.64	25.48	23.128

Analyze these data using the ANOVA method. Discuss whether the two-way blocking was useful. The means table for each individual treatment is as follow:

A	B	C	D	E
24.12	24.88	20.00	22.50	24.14

The model statement is as follow: $Y_{ijk} = \mu + \rho_i + \gamma_j + \tau_{(k)} + \epsilon_{ij}, i, j = 1, ..., 5, k \in 1, ..., 5$

- Y_{ijk} is the observation of the $i-th$ row, $j-th$ column subjected to the $k-th$ treatment.
- μ is the overall mean.
- ρ_i is the effect of the $i-th$ row.
- γ_j is the effect of the $j-th$ column.
- $\tau_{(k)}$ is the effect of the $k-th$ treatment.
- ϵ_{ij} is the random error.

The assumptions of the model are as follow:

1. $\rho_i \sim N(, \sigma_\rho^2)$.

2. $\gamma_j \sim N(0, \sigma_\gamma^2)$.
3. $\sum_k \tau_{(k)} = 0$.

The ANOVA Table is as follow:

Source	d.f.	SS	MS
Row	$p-1$	$p\sum_{i=1}^p(\bar{R}_i - \bar{Y})^2$	$SS(R)/(p-1)$
Column	$p-1$	$p\sum_{i=1}^p(\bar{C}_i - \bar{Y})^2$	$SS(C)/(p-1)$
Treatment	$p-1$	$p\sum_{i=1}^p(\bar{T}_i - \bar{Y})^2$	$SS(T)/(p-1)$
Error	$(p-1)(p-2)$		$SS(E)/[(p-1)(p-2)]$
Total	p^2-1		

Substituting in actual values into the ANOVA Table yields,

Source	d.f.	SS	MS	F	$p-$value
Row	4	18.2264	4.5566	0.78	0.5593
Column	4	1091.6664	272.9166	46.7219	0.0001
Treatment	4	76.2824	19.0706	3.2648	0.0498
Error	12	70.0952	5.8413		
Total	24	1256.2704			

The confidence intervals for the treatment means are as follow:

– Treatment A: $\bar{Y} \pm t_{0.025}(12)\sqrt{\frac{MSE}{p}} = 24.12 \pm \frac{2.179\sqrt{5.8413}}{\sqrt{5}} = [21.765, 26.475]$.

– Treatment B: $\bar{Y} \pm t_{0.025}(12)\sqrt{\frac{MSE}{p}} = 24.88 \pm \frac{2.179\sqrt{5.8413}}{\sqrt{5}} = [22.525, 27.235]$.

– Treatment C: $\bar{Y} \pm t_{0.025}(12)\sqrt{\frac{MSE}{p}} = 20.00 \pm \frac{2.179\sqrt{5.8413}}{\sqrt{5}} = [17.645, 22.355]$.

– Treatment D: $\bar{Y} \pm t_{0.025}(12)\sqrt{\frac{MSE}{p}} = 22.50 \pm \frac{2.179\sqrt{5.8413}}{\sqrt{5}} = [20.145, 24.855]$.

– Treatment E: $\bar{Y} \pm t_{0.025}(12)\sqrt{\frac{MSE}{p}} = 24.14 \pm \frac{2.179\sqrt{5.8413}}{\sqrt{5}} = [21.785, 26.495]$.

The standard error on the difference of two treatment means is given by, $\sqrt{\frac{2MS(E)}{p}} = \sqrt{\frac{2(5.8413)}{5}} = 1.529$. The confidence interval for two different treatment means is, $(\bar{Y}_k - \bar{Y}_{k'}) \pm 1.529$. The relative efficiency of columns as blocks and rows omitted is, $\frac{MS(R)+(p-1)MS(E)}{pMS(E)} = \frac{4.5566+4(5.8413)}{5(5.8413)} = 0.956$. Since $0.956 < 1$, column effects are not useful. The relative efficiency of rows as blocks and columns omitted is, $\frac{MS(C)+(p-1)MS(E)}{pMS(E)} = \frac{272.9166+4(5.8413)}{5(5.8413)} = 10.1444$. Since $10.1444 > 1$, row effects are useful. To compare the relative efficiency of the Latin square to a completely randomized design, the following equation is used: $\frac{MS(R)+MS(C)+(p-1)MS(E)}{(p+1)MS(E)} = \frac{4.5566+272.9166+(4)(5.8413)}{6(5.8413)} = 8.584$. Since $8.584 > 1$, the Latin square design is more efficient than a randomized block design. To test the F_1 statistic that all the mean effects are the same is as follow: $H_0 : \tau_1 = \tau_2 = \tau_3 = \tau_4 = \tau_5$ versus $H_1 : \tau_i \neq \tau_j, i \neq j, i, j \in 1, ..., 5$. $F_{0.05}(4, 12) = 3.26$. Since the observed $F_1 = 3.2648 > 3.26$ there is a significant different among treatments.

3. A company tested two chemistry methods for the determination of serum glucose. Three pools of serum were used for the experiment. Each pool contained different levels of glucose through the addition of glucose to the base level of an existing serum pool. Three samples of the serum from each pool were prepared independently for each level of glucose with each of the two chemistry methods. The concentrations of glucose (mg/dl) are

	Method 1			Method 2		
Glucose Level	1	2	3	1	2	3
	42.5	138.4	180.9	39.8	132.4	176.8
	43.3	144.4	180.5	40.3	132.4	173.6
	42.9	142.7	183.0	41.2	130.3	174.9
$\bar{Y}_{ij\cdot}$	42.90	141.83	181.47	40.43	131.70	175.10
$\bar{Y}_{i\cdot\cdot}$	122.07			115.74		
$\bar{Y}_{\cdot\cdot\cdot}$	118.905					

Analyze these data. This is a 2 factorial design.

8.17 2^k Factorial Designs

There are k factors with 2 levels for each factor. In general, there are 2^k treatments.

Example: A 2^3 design has 8 treatments. We are interested in the main effects, A, B, C, and the interactions AB, AC, BC, ABC.

Example: A 2^2 design.

Treatments	Replications
(1)	28, 25, 27
a	36, 32, 32
b	18, 19, 23
ab	31, 30, 29

Treatment	Total Yield
(1)	80
a	100
b	60
ab	90

The main effect of factor A is $A = \frac{90+100-60-80}{2r}$. Notation convention: the total yield at a particular treatment is denoted by the symbol of the treatment. Then, the main effect of A is $A = \frac{a+ab-b-(1)}{2r}$. The main effect of B is $B = \frac{ab+b-a-(1)}{2r}$. The main effect of AB is $AB = \frac{a+b-ab-(1)}{2r}$. Use a sign table to compute the above effects for larger designs.

	(1)	a	b	ab
A	-	+	-	+
B	-	-	+	+
AB	+	-	-	+

Example: A 2^2 design. The number of treatments is 4. Notation used: factor A: A_0, A_1, factor B: B_0, B_1. The treatments are $A_0B_0, A_0B_1, A_1B_0, A_1B_1$. These are denoted by (1), a, b, ab. Suppose there are r

replications,

Treatments				
(1)	1	2	...	r
a	1	2	...	r
b	1	2	...	r
ab	1	2	...	r

The main effects of factor A: $A = \frac{a+ab-b-(1)}{r2^{k-1}}$. The main effects of factor B: $B = \frac{b+ab-a-(1)}{r2^{k-1}}$. The main effects of interaction AB: $AB = \frac{ab+(1)-a-b}{r2^{k-1}}$. Note that:

1. The main effects and the interaction are simply certain contrasts of the total yields(or average yields).

2. The sum of squares of the factors and interaction are squares of the contrasts divided by appropriate quantities.

The sum of squares corresponding to factor A: $SS(A) = \frac{[a+ab-b-(1)]^2}{r2^2}$. The sum of squares corresponding to factor B: $SS(B) = \frac{[b+ab-a-(1)]^2}{r2^2}$. The sum of squares corresponding to interaction AB: $SS(AB) = \frac{[ab+(1)-a-b]^2}{r2^2}$. The ANOVA table for a 2^2 design:

Source	d.f.	SS	MS	F
Factor A	1	SS(A)	MS(A)	$\frac{MS(A)}{MS(E)}$
Factor B	1	SS(B)	MS(B)	$\frac{MS(B)}{MS(E)}$
Interaction AB	1	SS(AB)	MS(AB)	$\frac{MS(AB)}{MS(E)}$
Error	$2^2(r-1)$	SS(E)		
Total	$r2^2-1$			

H_0 : F_A significance of main factor A. F_B significance of main factor B. F_{AB} significance of interaction. SS(E) = SS(TOTAL) - SS(A) - SS(B) - SS(AB). Use Yate's algorithm to complete the contrasts:

Treatment	Total Yield	I	II	Effects	SS
(1)	(1)	a+(1)		—	—
a	a	b+ab	ab+a-b-(1)	$\frac{II}{r2^{2-1}}$	$\frac{SS(A)}{r2^2}$
b	b	a-(1)	b+ab-a-(1)	$\frac{II}{r2^{2-1}}$	$\frac{SS(B)}{r2^2}$
ab	ab	ab-a	ab+(1)-a-b	$\frac{II}{r2^{2-1}}$	$\frac{SS(AB)}{r2^2}$

8.17.1 Description of Yate's Algorithm

1. Write the treatment combinations in the standard order.

2. The response(total yield) is written in the next column. Then, the next k columns are formed as follow:

   (a) The first half of column I is obtained by adding the responses in the adjacent pairs. The second half of column I is obtained by changing the sign of the first entry in each of the pairs in the response column, and adding adjacent pairs.

   (b) Column II is obtained from column I as column I is obtained from the response column. Repeat until there are k columns.

3. The k-th column is the contrast for the effect designated at the beginning of the row. To get the estimate of effects, divide the entries in column k by $r2^{k-1}$. To get the sum of squares, divide the square of entries in column k by $r2^k$.

Example: $r = 3$ and $k = 2$.

Treatment	Total Yield	I	II	Estimate	SS
(1)	80	180	330	—	—
a	100	150	50	3.33	208.33
b	60	20	-30	-5	75
ab	90	30	10	1.67	8.33

Source	d.f.	SS	MS	F
A	1	208.33	208.33	53.15
B	1	75	75	19.13
AB	1	8.33	8.33	2.132
Error	8	31.34	3.92	
Total	11	323		

The null hypotheses corresponding to F_1 and F_2 are rejected since $F(1, 8) = 5.32$. F_3 is accepted. Therefore there is a difference between the two levels of factor A and the two levels in factor B.

Example: A 2^3 design. Factor A, % carbonation, has two levels: 10% and 12%. Factor B, pressure, has two levels: 25psi and 30psi. Factor C, line speed, has two levels: 200 and 250rpm. $r = 2$.

Treatment	Yield	I	II	III	SS
(1)	-4	-3	1	16	—
a	1	4	15	24	36
b	-1	2	11	18	20.25
ab	5	13	13	6	2.25
c	-1	5	7	14	12.25
ac	3	6	11	2	0.25
bc	2	4	1	4	1
abc	11	9	5	4	1

Source	d.f.	SS	MS	F
A	1	36	36	57.6
B	1	20.25	20.25	32.4
AB	1	2.25	2.25	3.6
C	1	12.25	12.25	19.6
AC	0.25	0.25	0.4	
BC	1	1	1	1.6
ABC	1	1	1	1.6
Error	8	5	0.625	
Total	15			

The levels of factors A, B, and C are significantly different. The interactions are insignificant. The completion of contrasts for 2^3 design using the *sign table* is as follow:

	(1)	a	b	ab	c	ac	bc	abc
A	−	+	−	+	−	+	−	+
B	−	−	+	+	−	−	+	+
AB	+	−	−	+	+	−	−	+
C	−	−	−	−	+	+	+	+
AC	+	−	+	−	−	+	−	+
BC	+	+	−	−	−	−	+	+
ABC	−	+	+	−	+	−	−	+

8.18 2^k Design with Blocking

There are k factors with two levels each. The number of treatments is 2^k. There are r replications. The number of experimental units is $r2^k$. The ANOVA table is as follow:

Source	d.f.	SS
A	1	Yate's
B	1	Yate's
AB	1	Yate's
C	1	Yate's
AC	1	Yate's
BC	1	Yate's
ABC	1	Yate's
Blocking	$r-1$	$2^k \sum_{i=1}^{r} (\bar{B}_i - \bar{y})^2$
Error	$(r-1)(2^k-1)$	
Total	$r2^k-1$	

$\bar{B}_i$ is the mean of the average yield in the i-th block. $\bar{y}$ is the overall mean.

8.19 Two Factor Factorial Design with $r = 1$

The model statement: $y_{ij} = \mu + \alpha_i + \beta_j + \epsilon_{ij}$. There is no interaction term because there would be no degrees of freedom for the error in the presence of an interaction term.

Source	d.f.	SS
Factor A	$a-1$	
Factor B	$b-1$	
Error	$(a-1)(b-1)$	
Total	$ab-1$	

A certain specific type of interaction(e.g. $(\alpha\beta)_{ij} = \lambda\alpha_i\beta_j$) are considered and tests for these are proposed in the literature.

8.20 2^k Design with $r = 1$

Even for a moderate number of factors($k = 5$), the total number of treatments is $2^5 = 32$. Even in a very simple situation of replications($r = 2$), 64 experimental units are required. Hence, in many cases only one replication is possible. In this case, the degrees of freedom of SS(E) is zero. *A remedy:* Assume that certain higher order interactions are negligible and the sums of squares of those interactions can be combined to get SS(E). *A few rules:*

1. Interactions which are to be pooled to get SS(E) are to be determined in advance.

2. If some higher order interactions are important, they can be retained.

3. As a general rule, it is usually safe to assume that 4 factor and higher interactions are negligible.

4. Two factor interactions should not be pooled.

5. The three factor interactions should be pooled only if necessary.

Example: A chemical product is produced in a pressured vessel. A factorial experiment is carried out in the pilot plant to study the factors thought to increase the filtration rate of the product. The four factors each with 2 levels are: A(temperature), B(pressure), C(concentration of formaldehyde), and D(stirring rate). A 2^4 design is used with $r = 1$.

Trts	Yield	I	II	III	IV	Est	SS
(1)	45	116	229	502	1121	–	–
a	71	113	273	619	173	21.625	1870.56
b	48	128	292	20	25	3.125	39.06
ab	65	145	327	155	1		0.06
c	68	143	43	14	79		390.06
ac	60	149	-23	11	-145		1314.06
bc	80	161	118	-16	19		22.56
abc	65	166	37	17	15		14.06
d	43	26	-3	44	117		85.56
ad	100	17	17	35	133		1105.56
bd	45	-8	6	-66	-3		0.56
abd	104	-15	5	35	33		68.06
cd	75	57	-9	20	-9		5.06
acd	86	59	-7	-7	-13		10.06
bcd	70	11	2	116	-21		27.56
abcd	96	26	15	15	11		7.56

A Q-Q plot of estimates of the contrasts of yield against the Normal distribution values is sometimes used to determine the treatments to pool to get SS(E). For illustration, along with ABCD, let's assume all third order interactions are negligible. The $SS(E) = 14.06+68.06+10.06+27.56+7.56$, with 5 degrees of freedom.

8.21 Homework and Answers

1. Complete the ANOVA Table and examine the test statistics from the problem done in class.

Trt	Yield	I	II	III	IV	Est
(1)	45	116	229	502	1121	—
a	71	113	273	619	173	21.625
b	48	128	292	20	25	3.125
ab	65	145	327	153	1	0.125
c	68	143	43	14	79	9.875
ac	60	149	-23	11	-145	-18.125
bc	80	161	116	-16	19	2.375
abc	65	166	37	17	15	1.875
d	43	26	-3	44	117	14.625
ad	100	17	17	35	133	16.625
bd	45	-8	6	-66	-3	-0.375
abd	104	-15	5	-79	33	4.125
cd	75	57	-9	20	-9	-1.125
acd	86	59	-7	-1	-13	-1.625
bcd	70	11	2	2	-21	-2.625
abcd	96	26	15	13	11	1.375

ANOVA Table

Source	d.f.	SS	MS	F
A	1	1870.56	1870.56	73.18*
B	1	39.06	39.06	1.528
AB	1	0.0625	0.0625	0.0024
C	1	390.06	390.06	15.26*
AC	1	1314.09	1314.06	51.41*
BC	1	22.56	22.56	0.88
D	1	855.56	855.56	33.47*
AD	1	1105.56	1105.56	43.25*
BD	1	0.56	0.56	0.022
CD	1	5.06	5.06	0.198
Error	5	127.81	25.56	
Total	15			*significant at 0.05

$F_{0.05}(1,5) = 6.61$. Recommendation: AC

Trt	Yield	I	II	Est
ac	-145	-66	1228	51.17
c	79	1294	1172	48.83
a	173	224	1360	56.67
(1)	1121	948	724	30.17

A	C −	C +
−	30.17	48.83
+	56.67	51.17

Recommend the low level of concentrate of formaldehyde(C) and the high level of temperature(A).
Recommendation: AD

Trt	Yield	I	II	Est
ad	133	250	1544	64.3
d	117	1294	932	38.83
a	173	-16	1044	43.5
(1)	1121	948	964	40.17

A \ D	−	+
−	40.17	38.83
+	43.5	64.3

Recommend the high level of the stirring rate(D).

2. An engineer is interested in the effects of cutting speed (A) toll geometry(B), and cutting angle(C) on the life(in hours) of a machine tool. Two levels of each factor are chosen, and three replicates of a 2^3 factorial design are run. The results are,

Treatments	(1)	a	b	ab	c	ac	bc	abc
I	22	32	35	55	44	40	60	39
II	31	43	34	47	45	37	50	41
III	25	29	50	46	38	36	54	47

a. Estimate the factor effects.

b. Use ANOVA for your analysis.

c. What levels of A,B, and C would you recommend?

Trt	Yield	I	II	III	Est	SS
(1)	78	182	449	980	81.67	—
a	104	267	531	4	0.33	0.667
b	119	240	55	136	11.33	770.67
ab	148	291	-51	-20	1.67	16.67
c	127	26	85	82	6.83	280.167
ac	113	29	51	-106	-8.83	468.17
bc	164	-14	3	-34	-2.83	48.167
abc	127	-37	-23	-26	-2.17	28.167

ANOVA Table

Source	d.f.	SS	MS	F
A	1	0.667	0.667	0.019
B	1	770.67	770.67	22.38*
AB	1	16.67	16.67	0.484
C	1	280.167	280.167	8.137*
AC	1	468.17	468.17	13.598*
BC	1	48.167	48.167	1.399
ABC	1	28.167	28.167	0.818
Blocking	2	0.583	0.2915	0.008
Error	14	482.069	34.43	
Total	23			*significant at 0.05

$F_{0.05}(1, 14) = 4.6$. Blocking was not effective. Recommendation: AC

Trt	Yield	I	II	Est
ac	-106	-24	960	40
c	82	984	1164	48.5
a	4	188	1008	42
(1)	980	976	788	32.83

A	C	
	$-$	$+$
$-$	32.83	48.5
$+$	42	40

Recommend the high level for the cutting edge(C) and the low level for the cutting speed(A). Recommendation: B

B	
$-$	$+$
35.17	46.5

Recommend the high level of the tool geometry(B).

3. In a process development study on yield, four factors were studied, each at two levels: time(A), concentration(B), pressure(C), and temperature(D). A single replicate of a 2^4 design was run, and the data follows:

Run No.	Run Order	A	B	C	D	Yield
1	5	-	-	-	-	12
2	9	+	-	-	-	18
3	8	-	+	-	-	13
4	13	+	+	-	-	16
5	3	-	-	+	-	17
6	7	+	-	+	-	15
7	14	-	+	+	-	20
8	1	+	+	+	-	15
9	6	-	-	-	+	10
10	11	+	-	-	+	25
11	2	-	+	-	+	13
12	15	+	+	-	+	24
13	4	-	-	+	+	19
14	16	+	-	+	+	21
15	10	-	+	+	+	17
16	12	+	+	+	+	23

Factor Levels		
	−	+
A(h)	2.5	3
B(%)	14	18
C(psi)	60	80
D(c)	225	250

Conduct an ANOVA analysis. Assume that 3rd and 4th level interactions are negligible.

8.22 Midterm Exam

1. In order to investigate whether eight different fats are absorbed in different amounts by a doughnut mix during cooking, batches of 24 doughnuts were cooked on six different days in each of the eight fats and the amount of fat absorbed was noted. Make an analysis of variance table and test the hypothesis that there is no difference among the mean amounts of fat absorbed when using the eight different fats.

   This is a RBD design.

2. Batches of ground meat from five different sources are charged consecutively into a rotary filling machine for packing into cans. The machine has six filling cylinders. Three filled cans are taken from each cylinder at random while each batch is being run. The weights of the filled cans are recorded. Write the analysis of variance table and give tests for testing various hypotheses.

   This is a 2-factor factorial design.

3. An ammunition manufacturer is studying the burning rate of power from three production processes. Four batches of power are randomly selected from the output of each process and three determinations of burning rate are made on each batch. Write a model for this data and give the ANOVA table.

   Model: $y_{ijk} = \mu + \tau_i + \beta_{ij} + \epsilon_{ijk}$. $p = 3, r = 4, n = 3$. This is a 2 stage nested, mixed model. The assumptions are:

   (a) $\epsilon_{ijk} \sim N(0, \sigma^2)$.
   (b) $\beta_{ij} \sim N(0, \sigma_\beta^2)$.
   (c) $\sum_{i=1}^{3} \tau_i = 0$.

   ϵ_{ijk} is the random error of the k-th sample in the j-th experimental unit of the i-th treatment. β_{ij} is the error in the j-th experimental unit of the i-th treatment. τ_i is the effect of the i-th treatment. μ is the overall mean.

ANOVA Table

Source	d.f.	SS	MS	F
Main Factor	2	$12\sum_{i=1}^{3}(\bar{y}_{i\cdot\cdot} - \bar{y}_{\cdot\cdot\cdot})^2$	$\frac{SS(MF)}{2}$	$\frac{MS(MF)}{MS(N)}$
Nesting	9	$3\sum_{i=1}^{3}\sum_{j=1}^{4}(\bar{y}_{ij\cdot} - \bar{y}_{i\cdot\cdot})^2$	$\frac{SS(N)}{9}$	$\frac{MS(N)}{MS(E)}$
Error	24	$\sum_{i=1}^{3}\sum_{j=1}^{4}\sum_{k=1}^{3}(y_{ijk} - \bar{y}_{ij\cdot})^2$	$\frac{SS(E)}{24}$	
Total	35	$\sum_{i=1}^{3}\sum_{j=1}^{4}\sum_{k=1}^{3}(y_{ijk} - \bar{y}_{\cdot\cdot\cdot})^2$		

4. In a one-way ANOVA model situation, suppose you have rejected the null hypothesis that effects of all the treatments is the same. As a subsequent analysis, you are asked to find the best treatment. Describe how you will find the best treatment by applying a multiple comparison procedure.

First look-up the $Q(\alpha, p, r)$ in a table. α is usually arbitrarily set at 0.05(level of significance). p is the number of treatments. r is the number of replications. Let's assume equal replication. If $|\bar{y}_{i\cdot} - \bar{y}_{j\cdot}| \geq Q(\alpha, p, r)\sqrt{\frac{MS(E)}{r}}$ for any $i, j \in 1, 2, ..., p$, then the two means are significantly different. The term MS(E) is the mean square of error from the ANOVA table. $\bar{y}_{i\cdot}$ and $\bar{y}_{j\cdot}$ are treatment means. This is known as Tukey's method for comparing means.

5. The effective life of a cutting tool installed in a numerically controlled machine is thought to be affected by the cutting speed and the tool angle. Three speeds and three angles are selected, and a factorial experiment with two replications is performed. The table below is part of the ANOVA table. Complete the table and test various hypotheses assuming both factors to be fixed.

Source	d.f.	SS	MS	F
Angle		24.33		
Speed		25.33		
Interaction		61.34		
Error				
Total		124.00		

The completed ANOVA table follows.

Source	d.f.	SS	MS	F
Angle	2	24.33	12.165	8.425
Speed	2	25.33	12.665	8.771
Interaction	4	61.34	15.335	10.62
Error	9	13.00	1.444	
Total	17	124.00		

F_3 :

$$H_0 : \gamma_{ij} = c, \forall i, j.$$

$$H_1 : \gamma_{ij} \neq c, \text{for at least one } (i, j) \text{ pair}$$

$F_{0.05}(4, 9) = 3.63$. Since $10.62 \geq 3.63$, H_0 is rejected.

F_2 :

$$H_0 : \beta_1 = \beta_2 = \beta_3.$$

$$H_1 : \beta_i \neq \beta_j, i, j \in 1, 2, 3.$$

$F_{0.05}(2, 9) = 4.26$. Since $8.771 \geq 4.26$, H_0 is rejected.

F_1 :

$$H_0 : \alpha_1 = \alpha_2 = \alpha_3.$$

$$H_1 : \alpha_i \neq \alpha_j, i, j \in 1, 2, 3.$$

Since $8.425 \geq 4.26$, H_0 is rejected.

8.23 An Example of 2^3 with Blocking

Example: A 2^3 design with 4 blocks. Use the data on page 172 of the text book.

Trts	Trts	Yields	I	II	III
(1)	(1)	425			9331
a	n	426			333
b	p	1283			2987
ab	np	1396			161
c	k	1118			2271
ac	nk	1203			105
bc	pk	1673			-669
abc	npk	1807			-63

Total(SS) = 466779.7 with $r2^k - 1 = 31$ degrees of freedom. $SS(BLOCK) = 2^k \sum_{i=1}^{r}(\bar{b}_i - \bar{y})^2 = 8\sum_{i=1}^{r}(\bar{b}_i - \bar{y})^2 = 774.1$, with $r - 1 = 3$ degrees of freedom. $\bar{y} = \frac{9331}{32} = 291.59$.
$\bar{b}_1, \bar{b}_2, \bar{b}_3, \bar{b}_4$ are averages of blocks 1, 2, 3, 4. Reference page 174, Table 8.8 for the final ANOVA table. PK is a significant interaction. N is independently significant. Hence, main effects P and K have no proper interpretation. In order to find the best level of P and K, we need to study the means table of P and K. The main effect N is significant and the best level of N can be obtained as follow:

	N	
	−	+
	0	50
mean yield	281.19	302.00

$\frac{4499}{16} = 281.19$, $\frac{9331-4499}{16} = 302$. Use 50lb of N. Next study P and K.

	K	
	0	20
0	106.38	290.13
20	334.88	435

Computation of the means using Yate's algorithm was as follow:

Trt	Old Col. III	I	II	Mean
pk	-669	1602	1392	435
k	2271	12318	9284	290.12
p	2987	2940	10716	334.88
(1)	9331	6344	3404	106.38

Recommend N at 50lb, K at 20lb, and P at 20lb.

8.24 Fractional Factorial Designs

We need 2^{k-p} fractions. There are r replications, r blocks of size 2^k. In applications, the size of the block is less than 2^k. If the number of experimental runs is less than the number of treatments, in a full factorial set, we have fractional replication leading to fractional factorial designs. Suppose we have 3 factors with 2 levels of each(2^3). We need $2^3 = 8$ experimental units. Suppose the number of experimental units is only 4.

Question: Which treatments from the set of 8 should be tested. Answer: We assume the abc interaction can definitely be ignored. Referencing the sign table, look at the signs for ABC. Arbitrarily choose a sign(+/−) and use those as experimental units.

+	−
a	(1)
b	ab
c	ac
abc	bc

Either of the two sets of treatments can be used in the experiment. A and BC have the same signs. We will not know where the differences are coming from. B and AC, C and AB are called *aliases.* We cannot separate the effects. They are equivalent. ABC cannot be estimated from the selected treatments. ABC is the *defining contrast.* If the contrasts are significant for A, there is no way of knowing whether it is really due to A or due to BC. Whenever a fractional replication design is used, every contrast has at least one or more other contrasts as an alias. Knowing that ABC is the defining contrast, either the + or the − treatments are used. Suppose (1), ab, bc, ac are used in the experiment. The following contrasts are aliases of each other.

Contrasts	Aliases
A	$\underline{A}(\underline{A}BC) = BC$
B	$\underline{B}(A\underline{B}C) = AC$
AB	$\underline{AB}(\underline{AB}C) = C$
C	$\underline{C}(AB\underline{C}) = AB$
AC	$\underline{AC}(\underline{A}B\underline{C}) = B$
BC	$\underline{BC}(A\underline{BC}) = A$
ABC	$\underline{ABC}(\underline{ABC}) = (1)$

When the contrast A is obtained, it measures the main effect of Factor A and the BC interaction.

8.24.1 Construction of $\frac{1}{2}2^k$ Design

Select a defining contrast, usually a higher order interaction. Then, use either those combinations which have a + sign or those with a − sign under the defining contrast. Choose a defining contrast such that:

1. No main effect has another main effect or no lower order interaction has a lower order interaction as aliases.

2. Some contrasts and their aliases are negligible so that they can be used as error.

Example: A $\frac{1}{2}2^4$ design. Take ABCD as the defining contrast.

+	−
(1)	a
ab	b
ac	c
bc	abc
ad	d
bd	abd
cd	acd
abcd	bcd

Use the + column. Suppose the yields are:

Treatments	Yields
(1)	550
ab	749
ac	1052
bc	650
ad	1075
bd	642
cd	641
abcd	729

Effect	Alias
A	BCD
B	ACD
AB	CD
C	ABD
AC	BD
BC	AD
ABC	D

8.24.2 Analysis of the Data

Since we are using 8 treatments, write the treatment combinations for a 2^3 design.

Trt	Yields	I	II	III	Effects+Aliases
(1)	550			6048	
a[d]	1075			-508	A + BCD
b[d]	642			16	B + ACD
ab	749			-40	AB + CD*
c[d]	601			46	C + ABD
ac	1052			-102	AC + BD*
bc	650			-790	BC + AD*
abc[d]	729			1162	ABC + D
					*error terms

Source	d.f.	SS	MS	F
A	1	32258	32258	1.22
B	1	32	32	0.001
C	1	264.5	264.5	0.01
D	1	168780.5	168780.5	6.368*
Error	3	79513	26504.33	

The error was calculated as follow: $SS(E) = \frac{(-40)^2}{8} + \frac{(102)^2}{8} + \frac{(790)^2}{8} = 79513$.

Example: Polymer coatings for aluminum cases. There are five factors:

- Factor A is two types of alloys.
- Factor B is two types of solvents.

- Factor C is two molecular structures of polymer coating.
- Factor D is two types of catalyst used in the adhesion process(10% and 15%).
- Factor E is two levels of curing temperatures(150° and 175°).

As a preliminary experiment, identify main effects and 2-factor interaction effects. A $\frac{1}{2}(2^5) = 2^{5-1}$ fractional factorial design was used. Use ABCDE as the defining contrast.

−	+
(1)	a
ab	b
ac	c
bc	abc
ad	d
bd	abd
cd	acd
abcd	bcd
ae	e
be	abe
ce	ace
abce	bce
de	ade
abde	bde
acde	cde
bcde	abcde

Suppose the treatments corresponding to + are used. The Yate's table is as follow:

Trts	Yield	I-III	IV	Alias+Effect
(1)[e]	41.5		725.2	—
a	39.6		-31.5	A+BCDE
b	43.9		-6.1	B+ACDE
ab[e]	38.8		-29.5	AB+CDE
c	48.7		77.6	C+ABDE
ac[e]	52.0		-3.3	AC+BDE
bc[e]	55.8		-0.7	BC+ADE
abc	43.2		3.5	ABC+DE
d	39.5		-2	D+ABCE
ad[e]	42.6		1.1	AD+BCE
bd[e]	44.0		-5.9	BD+ACE
abd	33.8		8.7	ABD+CE
cd[e]	53.6		6	CD+ABE
acd	48.1		1.3	ACD+BE
bcd	51.3		5.9	BCD+AE
abcd[e]	48.7		28.9	ABCD+E

$SS = \frac{[IV]^2}{2^4} = \frac{[IV]^2}{16}$.

8.24.3 Q-Q Plots

Use the *Q-Q plot* to identify the effects for finding SS(E) in the example in the previous section. Find the ordered effects of all the factors and main interaction. That is, find the ordered estimates from the column of contrasts. The estimates are computed as follow: $Est = \frac{[IV]}{r2^{k-1}} = \frac{[IV]}{8}$.

Example: Suppose $n = 15$. Then, $z_7 = \frac{7-\frac{1}{3}}{15+\frac{1}{3}} = 0.435 \Rightarrow z_7 = -0.16$. Then, plot $(-0.16, Q_7)$.

The ordered estimates are:

A	AB	B	BD	AC	D	BC	AD
-3.94	-3.69	-0.76	-0.74	-0.41	-0.24	-0.09	0.14

ACD	ABC	BCD	CD	ABD	E	C
0.16	0.44	0.74	0.75	1.09	3.61	9.71

If there are no significant effects, then the estimates are $N(0,1)$. Find $z_i, i = 1, 2, ..., 15$ such that $P\left(N(0,1) \leq z_i\right) = \frac{i-\frac{1}{3}}{n+\frac{1}{3}}, i = 1, 2, ..., 15$. Those points that do not lie on the line are significant. That is the 45° line. The points on the line can be used for SS(E). The ANOVA table is as follow:

Source	d.f.	SS	MS	F
A	1	62.02	62.02	44.11*
AB	1	54.39	64.39	38.68*
C	1	377.33	377.33	268.36*
E	1	52.20	52.20	37.13*
Error	11	15.47	1.406	
Total	15			*significant

Note: AB is significant, C and E are also significant. The means table for AB is

	B	
A	$-$	$+$
$-$	45.83	48.76
$+$	45.58	41.3

The means were obtained from the following Yate's table:

Trt	Old IV	I	II	Mean
ab	-29.5	-35.6	658.1	41.3
b	-6.1	693.7	780.1	48.76
a	-31.5	23.4	729.3	45.58
(1)	725.2	756.7	733.3	45.83

Recommend factor A with the first level and factor B with the 2-nd level. Recommend factor C with the second level since the estimate $9.71 > 0$. Factor D is insignificant. So recommend level 1 for economic reasons.

8.25 Confounding

Consider a 2^k design. Replications are possible. Blocking is needed to control the source of variability. But the block size is less than 2^k. (Remember, the block size is the number of experimental units in a block). Usually, we use all the treatments in a block. Such a design is a *complete block design.* If the size of the block is less than the number of treatments, then we have an incomplete block design. Assume that the block size(when 2^k treatments are available) is $\frac{1}{2}(2^k)$ or $\frac{1}{4}(2^k)$, etc. We need to identify an effect(usually a higher order interaction) which will confound with the block effect. Let ABCD be confounded with blocking. Recall the signs of this effect for different treatments with + sign one block and those with − sign the other block (assuming 2^4 design with 2 blocks per replication). Then, with 2 replications, there are 4 blocks, and the block size is 8. $SS(BLOCK) = 8\sum_{i=1}^{4}(\bar{b}_i - \bar{y})^2$, where $\bar{b}_1, ..., \bar{b}_4$ are the average yield of blocks 1 thru 4. $\bar{y}$ is the average of all the blocks. For the remaining sums of squares, use Yate's algorithm.

8.25.1 Partial Confounding

Recall a 2^3 design in 2 blocks(block size is 4) where ABC is confounded with the block effect. 4 replications are possible.

I		II		III		IV	
B1	B2	B3	B4	B5	B6	B7	B8
(1)	abc	(1)	abc	(1)	abc	(1)	abc
ac	a	ac	a	ac	a	ac	a
ab	b	ab	b	ab	b	ab	b
bc	c	bc	c	bc	c	bc	c

Note that the ABC effect is not being estimated. In this set-up, we can not estimate the ABC effect. However, we can design an experiment when there are replications so that the ABC effect can be estimated. Confound ABC, AB, BC, and AC for each replication. The design will be as follow:

I		II		III		IV	
B1	B2	B3	B4	B5	B6	B7	B8
(1)	abc	(1)	a	(1)	b	(1)	a
ab	a	c	b	a	c	b	c
ac	b	ab	ac	bc	ab	ac	ab
bc	c	abc	bc	abc	ac	abc	bc

Note that 3 out of 4 replications are used for ABC. The information about estimating the ABC effect can be obtained from replications II, III, IV. This design is said to be *partially confounded.*

Source	d.f.	Relation	SS
Blocking	7	—	$4\sum_{i=1}^{r}(\bar{b}_i - \bar{y})^2$
A	1	1	Yate's
B	1	1	Yate's
AB	$1'$	$\frac{3}{4}$	SS(AB)
C	1	1	Yate's
AC	$1'$	SS(AC)	
BC	$1'$	SS(BC)	
ABC	$1'$	SS(ABC)	
Error	17	—	Deduce
Total	31		

The general Yate's table follows:

Trt	Total Yield	I-III	SS
(1)			—
a			SS(A)
b			SS(B)
ab			No good
c			SS(C)
ac			No good
bc			No good
abc			No good

Note:

1. Calculate the unconfounded main effects using all the data as shown.

2. Contrasts confounded interactions are calculated as follow: Find the total yields from the replications where the treatment is unconfounded (e.g. AB from I, III, IV). $T_1 = \sum_{i=1}^{3}(1)$, $T_a = \sum_{i=1}^{3} a$, $T_b = \sum_{i=1}^{3} b$, ...etc. Then, using the sign table for AB, $AB = T_1 - T_a - T_b + T_{ab} + T_c - T_{ac} - T_{bc} + T_{abc}$. Then, $SS(AB) = \frac{[AB]^2}{3(2^k)}$, where the 3 is the actual replications due to confounding.

Example: A 2^3 design with partial confounding, 2 replications, and block size equal to 4.

I		II	
B1	B2	B3	B4
(1) [-3]	a [0]	(1) [-1]	a [1]
ab [2]	b [-1]	c [0]	b [0]
ac [2]	c [-1]	ab [3]	ac [1]
bc [1]	abc [6]	abc [5]	bc [1]

The Yate's table is:

Trt	Yields	I-II	III	SS
(1)	-4		16	—
a	1		24	36
b	-1		18	20.25
ab	5		6	No good
c	-1		14	12.25
ac	3		2	0.25
bc	2		4	1
abc	11		4	No good

Compute SS(AB): $AB = -3 - 0 + 1 + 2 - 1 - 2 - 1 + 6 = 2$. Then, $SS(AB) = \frac{2^2}{1(2^3)} = 0.5$. Compute SS(ABC): $ABC = 1 + 0 + 0 + 5 - 3 - 1 - 1 + 1 = 2$. Then, $SS(ABC) = \frac{2^2}{1(2^3)} = 0.5$ The ANOVA table is:

Source	d.f.	SS	Relation	MS	F
Blocks	3	3.5	—	1.17	1.56
A	1	36	1	36	48*
B	1	20.25	1	20.25	27*
AB	$1'$	0.5	$\frac{1}{2}$	0.5	0.67
C	1	12.25	1	12.25	16.33*
AC	1	0.25	1	0.25	0.33
BC	1	1	1	1.33	
ABC	$1'$	0.5	$\frac{1}{2}$	0.5	0.67
Error	5	3.75	—	0.75	
Total	15	78			*significant

Since $1.56 > 1$, blocking was effective. Only the main effects are significant.

8.26 BIBD Design

Suppose there are a treatments and the block size is $k < a$. Then, we have an incomplete block design. When confounding is used, we are in fact working with an incomplete block design. We have seen that using partial confounding, estimates of confounded contrasts are estimated using fractional information. Question: Are there any designs(incomplete block designs) which will allow us to estimate all the effects with equal precision? A partial answer to this is a design called *Balanced Incomplete Block Design(BIBD).* When all the treatment comparisons(pairwise) are equally important(equal precision), the treatment combinations used in each block should be selected in a balanced manner, such that any pair of treatments occur the same number of times as another pair. A BIBD is an incomplete block design in which any two treatments appear together an equal number of times.

Example: Block size is $k = 2$. There are 3 treatments A, B, C. The treatment pairs are (A,B), (A,C), (B,C). Thus $a = 3$. The number of blocks $b = 3$.

1	2	3
A	A	B
B	C	C

Note that the number of replications, $r = 2$. The number of times each pair occurs is $\lambda = 1$. The total number of experimental units is $ar = bk$. In general, $\lambda = \frac{r(k-1)}{a-1}$. λ must be an integer.

Example: The number of treatments is 3, (A,B,C).

1	2	3	4	5	6
A	A	B	A	A	B
B	C	C	C	B	C

$a = 3$, $b = 6$, $k = 2$, $r = 4$, $\lambda = \frac{4(1)}{2} = 2$.

Example: The number of treatments is 4, (A,B,C,D). The block size is 2. Then, 6 blocks are needed, (AB), (AC), (AD), (BC), (BD), (CD). The number of replications is 3 because A has been tried 3 times, for example.

Example: There are 4 treatments and the block size is 3.

1	2	3	4
A	A	A	B
B	B	C	C
C	D	D	D

$a = 4$, $k = 3$, $b = 4$, $\lambda = 2$, $r = 3$ because A occurs 3 times, for example. $\lambda = \frac{3(2)}{3} = 2$.

Example: Suppose there are a treatments and the block size is k. Suppose $k < a$. A BIBD can be constructed by taking $\begin{pmatrix} \mathrm{a} \\ \mathrm{k} \end{pmatrix}$ blocks and assigning a different combination of treatments to each block.

Example: $a = 4$, $k = 3$. The number of blocks is given by, $\begin{pmatrix} 4 \\ 3 \end{pmatrix} = \frac{4!}{3!} = 4$. The combinations are (ABC), (ABD), (ACD), (BCD). The balance in a BIBD can be obtained with fewer than $\begin{pmatrix} \mathrm{a} \\ \mathrm{k} \end{pmatrix}$ blocks. Tables of BIBD's for different choices of a and k are available in many text books. See Cocharan and Cox, 1957 or Fisher and Yates, 1953.

8.26.1 Analysis of the Data

Data:

	Blocks			
A	$\surd$	$\surd$	$\surd$	
B	$\surd$	$\surd$		$\surd$
C	$\surd$		$\surd$	$\surd$
D		$\surd$	$\surd$	$\surd$

Analysis must be done using a linear model but for unbalanced data. Suppose there are a treatments, the block size is k, the number of replications is r, and the number of blocks is b. Then, the number of experimental units is ar or bk. Model: $y_{ij} = \mu + \tau_i + \beta_j + \epsilon_{ij}$. τ_i is the effect of the i-th treatment, β_j is the effect of the j-th block, and $\epsilon \sim N(0, \sigma^2)$. The decomposition of the total sum of squares is given by: $\sum_i \sum_j (y_{ij} - \bar{y})^2 = k \sum_{j=1}^{b} (\bar{y}_{\cdot j} - \bar{y})^2 + \frac{k}{\lambda a} \sum_{i=1}^{a} Q_i^2 + SS(E)$. SS(E) is deduced by subtraction. SS(TRT) adjusted for blocking: Each treatment is represented in a different set of r blocks. $SS(TRT) = \frac{k}{\lambda a} \sum_{i=1}^{a} Q_i^2$, where $Q_i = y_{i\cdot} - \frac{1}{k} \sum_{j=1}^{b} n_{ij} y_{\cdot j}, i = 1, 2, ..., a$. $y_{i\cdot}$ is the sum of the i-th treatment. $y_{\cdot j}$ is the sum of the j-th block. $n_{ij} = 1$ if treatment i appears in block j, zero otherwise. The total degrees of freedom is given by $n - 1 = (b - 1) + (a - 1) + (n - a - b + 1)$. The last set represents degrees of freedom of the error. The SAS code is

```
INPUT TRT $ BLOCK $ Y;

...

PROC GLM;
CLASSES TRT BLOCK YIELD;
MODEL Y=TRT BLOCK;
RUN;
```

Example: Illustrate analysis of data using BIBD. The number of treatments is $a = 4$. The number of blocks is $b = 4$. The block size is $k = 3$. Data:

	Blocks				
	1	2	3	4	$y_{i\cdot}$
A	73	74	—	71	218
B	—	75	67	72	214
C	73	75	68	—	216
D	75	—	72	75	222
$y_{\cdot j}$	221	224	207	218	870

The number of replications $r = 3$. λ is the number of times a pair of treatments occurs. $\lambda = \frac{r(k-1)}{a-1} = \frac{3(2)}{3} = 2$. n is the total number of observations. $n = 12$. $SS(TOTAL) = \sum_i \sum_j (y_{ij} - \bar{y})^2 = 81$. $SS(BLOCK) = k\sum_{i=1}^{4}(\bar{y}_{\cdot j} - \bar{y})^2 = 55$. $SS(TRT) = \frac{k}{\lambda a}\sum_{i=1}^{4} Q_i^2$, $Q_1 = 218 - \frac{1}{3}(221 + 224 + 218) = -\frac{9}{3} = -3$. $Q_2 = -\frac{7}{3}$. $Q_3 = -\frac{4}{3}$. $Q_4 = \frac{20}{3}$. Then, $SS(TRT) = 22.75$. $SS(E) = SS(TOTAL) - SS(BLOCK) - SS(TRT) = 81 - 55 - 22.75 = 3.25$, with $11 - 3 - 3 = 5$ degrees of freedom. The ANOVA table is

Source	d.f.	SS	MS	F	p
Block	3	55	18.33	28.21	—
Trt(adjusted)	3	22.75	7.58	11.67	0.0107*
Error	5	3.25	0.65		
Total	11	81			

Since $28.21 > 1$, blocking was effective. The treatment effects are significantly different. Reject $H_0 : \tau_1 = \tau_2 = \tau_3 = \tau_4$. Special SAS note: Use `PROC GLM` to find SS(TRT) under Type III sums of squares. But, for SS(BLOCK), find it under Type I sums of squares.

8.27 Split Plot Design

Suppose treatment A has a levels and treatment B has b levels. Then, ab treatments are being crossed. Each plot is split into b parts.

A_1	A_2	...	A_a
B_1	B_1	...	B_1
B_2	B_2	...	B_2
.	.	.	.
.	.	.	.
.	.	.	.
B_b	B_b	...	B_b

In the split plot design, the levels of one factor are assigned at random to large experimental units called *whole plots.* The large experimental units are divided into smaller units called *sub plots.* The levels of the second factor are assigned at random to the small units within the whole plot.

8.27.1 Analysis of the Data

Model: $y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + B_k + \epsilon_{ijk} + \omega_{ik}, k = 1, 2, ..., r, i = 1, 2, ..., a, j = 1, 2, ..., b$. $\epsilon_{ijk} \sim N(0, \sigma^2)$. $\omega \sim N(0, \sigma_\omega^2)$. The hypotheses tests are: $H_{0A} : \alpha_1 = \alpha_2 = \cdots = \alpha_a$. $H_{1A} : \alpha_i \neq \alpha_j, i, j \in 1, 2, ..., a$. $F = \frac{MS(A)}{MS(1)}$. $H_{0B} : \beta_1 = \beta_2 = \cdots = \beta_b$. $H_{1B} : \beta_i \neq \beta_j, i, j \in 1, 2, ..., b$. $F = \frac{MS(B)}{MS(2)}$ $H_{0AB} : (\alpha\beta)_{ij} = \gamma$.

$H_{1AB} : (\alpha\beta)_{ij} \neq \gamma$. $F = \frac{MS(AB)}{MS(2)}$. The decomposition of the sums of squares is as follow: $SS(TOTAL) = \sum_i \sum_j \sum_k (y_{ijk} - \bar{y})^2$ with $abr - 1$ degrees of freedom. $SS(BLOCK) = ab\sum_{k=1}^{r}(\bar{y}_{\cdot\cdot k} - \bar{y})^2$ with $r - 1$ degrees of freedom. $SS(A) = br\sum_{i=1}^{a}(\bar{y}_{i\cdot\cdot} - \bar{y})^2$ with $a - 1$ degrees of freedom. $SS(B) = ar\sum_{j=1}^{b}(\bar{y}_{\cdot j\cdot} - \bar{y})^2$ with $b - 1$ degrees of freedom. $SS(E1) = b\sum_i \sum_k (\bar{y}_{i\cdot k} - \bar{y}_{i\cdot\cdot} - \bar{y}_{\cdot\cdot k} + \bar{y})^2$ with $(r - 1)(a - 1)$ degrees of freedom. $SS(AB) = \sum_i \sum_j (\bar{y}_{ij\cdot} - \bar{y}_{i\cdot\cdot} - \bar{y}_{\cdot j\cdot} + \bar{y})^2$ with $(a - 1)(b - 1)$ degrees of freedom. $SS(E2) = SS(TOT) - SS(BLK) - SS(A) - SS(B) - SS(AB) - SS(E1)$ with $a(b-1)(r-1)$ degrees of freedom. The SAS code is as follow:

```
INPUT A $ B $ BLOCK $ Y;

...

PROC ANOVA;
CLASSES A B BLOCK;
MODEL Y=A B A*B BLOCK BLOCK*A;
TEST H=A BLOCK E=BLOCK*A;
RUN;
```

Example: Green turf(golf) experiment. Factor A has 4 levels: Nitrogen, Urea, AS, IBDV, SC. Factor B is time with 3 levels: 2 years, 5 years, 8 years. There are 2 blocks.

Block 1

3.8	5.2	6.0	6.8
5.3	5.6	5.6	8.6
5.9	5.4	7.8	8.5

Block 2

3.9	6.0	7.0	7.9
5.4	6.1	6.4	8.6
4.3	6.2	7.8	8.4

The ANOVA table is as follow:

Source	d.f.	SS	MS	F
Block	1	0.5104	0.5104	1.22
Factor A	3	37.3246	12.442	29.673
Error 1	3	1.2579	0.4193	
Factor B	2	3.8158	1.9079	8.89
Factor AB	6	4.1502	0.6917	3.23
Error 2	8	1.7167	0.215	
Total	23			

Since $1.22 > 1$, blocking was effective. The means table for AB is

	Factor B		
	2	5	8
U	3.85	5.35	5.1
AS	5.6	5.85	5.8
IBDV	6.5	6.0	7.8
SC	7.35	8.6	8.45

Recommend SC for 5 years.

8.27.2 Repeated Measures Data

Many experiments have more than one observation on the same individuals. This leads to repeated measurements. The data is correlated(not an iid sequence). Factor A is the individuals and Factor B is time periods. Model: $y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + B_k + \omega_{ik} + \epsilon_{ijk}$. α_i is the effect of the i-th level of factor A. β_j is the effect of the j-th level of time. $(\alpha\beta)_{ij}$ is the interaction of level i of A with level j of B. $Cov(y_{111}, y_{121}) = Cov(\omega_{11} + \epsilon_{111}, \omega_{11} + \epsilon_{121}) = Cov(\omega_{11}, \omega_{11}) = Var(\omega_{11}) = \sigma_\omega^2$. The correlation coefficient of (y_{111}, y_{121}) is $\rho = \frac{Cov(y_{111},y_{121})}{\sqrt{Var(y_{111})Var(y_{121})}} = \frac{\sigma_\omega^2}{\sigma_\omega^2+\sigma^2}$ because $Var(y_{ijk}) = \sigma_\omega^2 + \sigma^2$. $0 \le \rho \le 1$ is the *intra-class correlation coefficient.*

8.27.3 Cross-over Trials

Used in clinical trials where human subjects are involved. The crossover study describes experiments with treatments administered in sequence to each experimental unit. A treatment is administered to an experimental unit for a specific period of time after which another treatment is administered to the same experimental unit. The treatments are successively administered to the unit until it has received all treatments.

Example: Suppose there are 3 treatments, A, B, C. For a cross over design, 6 subjects are needed to run all 6 possible sequences of the treatments. They are ABC, ACB, BCA, BAC, CAB, CBA. 3 time periods(or wash out periods) are needed.

8.27.4 AB/BA Design

This is a simple 2×2 design. A group of n_1 subjects is given treatment A and after a wash-out period, treatment B. A group of n_2 subjects is given treatment B and after a wash-out period, treatment A.

Period 1	Period 2
A(y_{iAP_1})	B(y_{iBP_2})
B(x_{iBP_1})	A(x_{iAP_2})

Paired T-test

The paired T-test is used to test the following hypothesis: $H_0 : \mu_A = \mu_B$ versus $H_1 : \mu_A \neq \mu_B$. It is assumed that there is no time period effect. An estimate of $\mu_A - \mu_B$ is $\frac{(\bar{y}_{AP_1} - \bar{y}_{BP_2}) + (\bar{x}_{AP_2} - \bar{x}_{BP_1})}{2}$. $\bar{y}_{AP_1} = \frac{1}{n_1}\sum_{i=1}^{n_1} y_{iAP_1}, etc...$ The standard error of the estimate is given by $\frac{1}{2}\hat{\sigma}\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}$, $\hat{\sigma}$ is the pooled standard deviation using the differences of the data from the two groups. $t = \frac{\hat{\mu}_A - \hat{\mu}_B}{SE} \sim t(n_1 + n_2 - 1)$.

Data Analysis with Time Period Effects

In this case, $E(y_{iAP_1}) = \mu_A + \mu_{P_1}$. $E(y_{iBP_2}) = \mu_B + \mu_{P_2}$. $E(x_{iBP_1}) = \mu_B + \mu_{P_1}$. $E(x_{iAP_2}) = \mu_A + \mu_{P_2}$. The hypothesis test is $H_0 : \mu_A - \mu_B = 0$ versus $H_1 : \mu_A - \mu_B \neq 0$. For group 1: $E(y_{iAP_1}) - E(y_{iBP_2}) = \mu_A - \mu_B + \mu_{P_1} - \mu_{P_2}$. For group 2: $E(x_{iAP_2}) - E(x_{iBP_1}) = \mu_A - \mu_B + \mu_{P_2} - \mu_{P_1}$. Let $n_1 = n_2$. Let $D_i = (y_{iAP_1} - y_{iBP_2}) + (x_{iAP_2} - x_{iBP_1}) = E\left(\frac{D_i}{2}\right) = (\mu_A - \mu_B)$. The t-test is $t = \frac{\frac{\bar{D}}{2}}{\text{SE of } \frac{\bar{D}}{2}} \sim t_{\alpha/2}(n-1)$. $H_0 : \mu_{P_1} - \mu_{P_2} = 0$ versus $H_1 : \mu_{P_1} - \mu_{P_2} \neq 0$. Use, $(y_{iAP_1} - y_{iAP_2}) - (x_{iAP_2} - x_{iBP_1})$.

8.28 Homework

1. Consider a 2^{5-1} fractional factorial design with ABCDE as the defining contrast. The data obtained are $e = -0.63$, $a = 2.51$, $b = -2.68$, $abe = 1.66$, $c = 2.06$, $ace = 1.22$, $bce = -2.09$, $abc = 1.93$, $d = 6.79$, $ade = 5.47$, $bde = 3.45$, $abd = -2.0$, $cde = 5.22$, $acd = 4.38$, $bcd = 4.30$, and $abcde = 4.05$. Find the aliases of variance contrasts and analyze the data.

2. An experiment was conducted to investigate the effects of four factors on the operation of a metal lathe. The four factors each at two levels were A: speed of the lathe rotation(60, 75); B: angle of cut(30, 45); C: frequency of lubrication(10sec, 30sec); D: alloy for cutting tip(1 and 2). The factor levels were used in a 2^4 factorial arrangement for the experiment. Only eight cutting trials could be run in a single day. An incomplete block design with two blocks(days) in each of two replications was set up with ABCD effect confounded with the block effect. The cutting tip wear for each of the treatments in each block are

Replication I		Replication II	
Day 1	Day 2	Day 3	Day 4
(1)(40)	a(24)	(1)(43)	a(28)
ab(33)	b(31)	ab(30)	b(35)
ac(31)	c(27)	ac(30)	c(28)
bc(38)	abc(23)	bc(32)	abc(20)
ad(22)	d(48)	ad(26)	d(44)
bd(37)	abd(35)	bd(33)	abd(36)
cd(49)	acd(29)	cd(40)	acd(25)
abcd(30)	bcd(37)	abcd(31)	bcd(34)

Compute the ANOVA table and interpret the results.

3. An animal scientist conducted a study on the effect of heat stress and dietary intake of protein and saline water on laboratory mice. The three factors were each used at two levels in a 2^3 factorial arrangement. The levels for the factors were A: protein(low, high); B: water(normal, saline); C: heat stress(room temperature, heat strength). An incomplete block design was used with four mice from an individual litter used in each block. Each mouse was put in an individual cage and assigned one of the treatments. One replication of the experiment consisted of two litters of mice. The weight gains(grams) for the mice are shown below.

Replication I		Replication II		Replication III	
Litter 1	Litter 2	Litter 3	Litter 4	Litter 5	Litter 6
(1)(27.5)	ab(24.3)	bc(19.5)	abc(19.7)	(1)(24.5)	a(33.1)
bc(20.6)	c(24.3)	a(24.1)	b(19.5)	c(23.0)	b(20.5)
abc(22.0)	ac(22.8)	ab(22.4)	(1)(22.5)	ab(23.4)	ac(19.8)
a(28.6)	b(24.6)	c(22.0)	ac(18.8)	abc(21.7)	bc(18.5)

Compute the ANOVA table and interpret the results.

8.29 Homework and Answers

1. The addition of acetylene to methyl glucoside in the presence of a base under high pressure had been found to result in the product of several mono-vinyl ethene; a process known as vinylation. The chemists wanted to obtain more specific information about the effect of pressure on percent conversion of methyl glucoside to mono-vinyl isomers. Five pressures: 250, 325, 400, 475, and 500psi were used. Only three high-pressure chambers were available for one run of the experimental conditions.

It was necessary to block on runs because there could be substantial run to run variation produced by new setups of the experiment in the high-pressure chambers. The chemists set up a BIBD with ten blocks(runs) each with three experimental units(pressurized chambers). The percent conversion of methyl glucoside by acetylene under pressure:

	Pressure				
Run	250	325	400	475	550
1	16	18	—	32	—
2	19	—	—	46	45
3	—	26	39	—	61
4	—	—	21	35	55
5	—	19	—	47	48
6	20	—	33	31	—
7	13	13	34	—	—
8	21	—	30	—	52
9	24	10	—	—	50
10	—	24	31	37	—

Analyze these data.

Source	d.f.	SS	MS	F
Block	9	1394.67	154.96	5.02
Trt(adjusted)	4	3688.578	922.1445	29.90
Error	16	493.422	30.84	
Total	29			

2. A split-plot experiment was conducted on sorghum with two treatment factors, plant population density and hybrid. The whole plots were used for the four levels of plant population density: 10, 15, 25 and 40 plants per meter of soil. There were three hybrids randomly allocated to the subplots of each plot. The experiment was conducted in a randomized complete block design with four replications. The data follows.

		Plants per Meter			
Hybrid	Block	10	15	25	40
TAM680	1	40.7	24.2	16.1	11.2
	2	37.8	44.4	17.6	12.7
	3	32.9	27.8	19.9	14.5
	4	43.1	34.1	20.1	15.4
RS671	1	39.4	31.3	17.9	14.8
	2	47.8	34.5	30.5	17.3
	3	44.4	25.6	22.5	17.7
	4	49.0	50.4	25.4	18.7
399x2536	1	68.7	26.2	20.5	18.9
	2	56.2	48.1	28.2	26.2
	3	44.8	41.1	30.0	19.2
	4	59.3	46.0	24.7	22.0

Analyze these data.

Source	d.f.	SS	MS	F
Factor A	3	6426.1675	2142.06	41.41
Blocks	3	410.2575	136.75	2.64
Error 1	9	465.5075	51.72	—
Factor B	2	881.26	440.63	17.74
Interaction AB	6	208.171	34.7	1.40
Error 2	24	595.96	24.83	—
Total	47			

8.30 Final Exam

1. For a split-plot design:

   (a) Describe the design.

   (b) Write the linear model.

   (c) Write down all the hypotheses of interest.

   (d) Present the ANOVA table to test the hypotheses.

2. The following data are obtained using a balanced incomplete block design(BIBD). Identify all the constants of the design and analyze these data.

	Block							
Trt	1	2	3	4	5	6	7	Total
1	11	—	—	—	12	—	11	34
2	12	12	—	—	—	11	—	35
3	—	13	11	—	—	—	13	37
4	14	—	12	14	—	—	—	40
5	—	14	—	15	14	—	—	43
6	—	—	12	—	11	12	—	35
7	—	—	—	13	—	13	12	38
Total	37	39	35	42	37	36	36	262

   The total sums of squares is 29.2381 with 20 degrees of freedom. Further, $Q_1 = -2.67$, $Q_2 = -2.33$, $Q_3 = 0.33$, $Q_4 = 2$, $Q_5 = 3.67$, $Q_6 = -1$, and $Q_7 = 0$.

3. Consider the following data where a partial confounding was used. Analyze these data.

I		II	
1	2	3	4
(1)(-3)	a(0)	(1)(-1)	b(0)
ab(2)	b(-1)	a(1)	ab(3)
ac(2)	c(-1)	bc(1)	c(0)
bc(1)	abc(6)	abc(5)	ac(1)
ABC confounded		BC confounded	

   The total sum of squares is 78.00 with 15 degrees of freedom.

4. A fisherman has conducted a 2^4 factorial design to determine the effects of four factors on the number of fish he catches in a four hour period. The variables studied and their levels for the experiment are

Factor	Low Level	High Level
Fishing location	Pier	Boat
Bait type	Worms	Night crawlers
Time of day	Day	Night
Weather	No rain	Rain

The results of the experiment given in the *standard order* are: 25, 26, 31, 34, 24, 26, 32, 36, 30, 36, 40, 43, 30, 34, 40, 42. Column IV of the Yate's table is: 529, 67, –1, –1, –5, 5, 1, 61, 5, 3, –9, –5, –1, –3, 1.

(a) Calculate estimates of all the effects.

(b) Construct ANOVA(to identify the best levels of the factors) assuming negligible higher order interactions.

(c) Construct a 95% confidence interval for the main effect of weather.

5. Consider a 2^{4-1} fractional factorial design with ABCD as the defining contrast. Write the treatment combinations to be run in the experiment. Write alias pattern for this design and describe how you will conduct the analysis of the data.

6. Construct one replication of(an incomplete block design) a 2^4 factorial design in two blocks of eight experimental units each with ABCD confounded with blocks.

7. Suppose two replications of a 2^4 factorial experiment is required. The design must be conducted with blocks of size eight. Construct a design such that no effect is completely confounded with blocks in the experiment.

8. A study was conducted on human subjects to measure the effects of three foods on serum glucose levels. Each of the three foods was randomly assigned to four subjects. The serum glucose was measured for each of the subjects at 15, 30, and 45 minutes after the food was ingested. Indicate how you would analyze data coming from such a study.

9. Three brands of batteries are under study. It is suspected that the lives(in weeks) of the three brands are different. Five batteries of each brand are tested and data are obtained. How do you analyze these data?

10. An experiment in soil microbiology was conducted to determine the effect of nitrogen fertility on nitrogen fixation by Rhizobium bacteria. The experiment was conducted with four crops: alfalfa, soybeans, guars and mugbean. Two plants were inoculated with the Rhizobium and grown in a Leonard jar with one of three rates of nitrogen in the media: 0, 50, or 100ppm N. Four replications, Leonard jars, were used for each of the 12 treatment combinations. The treatments were arranged in a completely randomized design in a growth chamber. The acetylene reduction was measured for each treatment when the plants were at the flowering stage. Acetylene reduction reflects the amount of nitrogen that is fixed by the bacteria in the symbiotic relationship with the plant. Write a linear model to analyze these data and write the ANOVA table.

Chapter 9

Nonparametric Statistics

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Statistics 549, Fall 1996
Text used: Lehmann, Statistical Methods Based on Ranks.

9.1 Rank Tests for Comparing 2 Treatments

9.1.1 Untied Observations

Non-parametric statistics is used when the Normality assumption does not hold true. The *Wilcoxon Rank Sum Test* is used to:

1. Compare a new treatment with a control or standard treatment.
2. Compare two new treatments to decide which treatment is better.

The hypotheses tests are: H_0 : No treatment effect(ie no systematic differences between treatment and control responses). H_1 : The treatment responses tend to be larger than the control responses. OR H_1 : The treatment responses tend to be smaller than the control responses. *Randomization Model:* A given set of N subjects is randomly divided into a set of size n who will receive the new treatment and a group of size $m(N = m + n$ which is the combined sample size) to be treated by a standard method. *Each subset of size n is equally likely to be assigned to the treatment groups.* The notation used is as follow:

- $x_1, x_2, x_3, ..., x_n$ are the control responses.
- $y_1, y_2, y_3, ..., y_n$ are the treatment responses.
- $S_1, S_2, S_3, ..., s_n$ are the treatment ranks.
- $R_1, R_2, R_3, ..., R_n$ are the control ranks.

Tip: Underline either $x's$ or $y's$ for easy calculation. $W_S = S_1 + S_2 + \cdots + S_n$ which is the sum of the treatment ranks. $W_R = R_1 + R_2 + \cdots + R_n$ which is the sum of the control ranks. To calculate the rank statistic:

1. Form the combined set of $N = n + m$ observations.
2. Assign the smallest value in this set a rank of 1, the next largest a rank of 2, etc.
3. The total set of ranks assigned is $1, 2, 3, ..., N$.
4. W_S is the sum of ranks of observations in the treatment group which is the sum of a subset of $\{1, 2, ..., N\}$.

The null distribution of the treatment ranks: the n-tuple $(S_1, S_2, ..., S_n)$ of treatment ranks is a subset of the total set of ranks $\{1, 2, ..., N\}$. Under H_0, this n-tuple is distributed as a sample size n taken without replacement from a finite population $\{1, 2, ..., N\}$. That is, $P_{H_0}(S_1 = s_1, S_2 = s_2, ..., S_n = s_n) = \frac{1}{\binom{N}{n}}$.

Under H_a, $(S_1, S_2, ..., S_N)$ will tend to take larger of smaller values than predicted by H_0.

Example: To determine whether discouragement adversely affects performance on an intelligence test, 10 subjects were randomly assigned into control and treatment groups of size 5 each. Each subject was given form L of the test and then 2 weeks later given form F of the test. The treatment group was subjected to conditions of discouragement. The score(mean) recorded for each subject was score equals later score minus original score. Controls: 5, 0, 16, 2, 9. Treatments: 6, –5, –6, 1, 4. The combined ordered set is:

Ordered set:	$\underline{-6}$	$\underline{-5}$	0	$\underline{1}$	2	$\underline{4}$	5	$\underline{6}$	9	16
Ranks:	1	2	3	4	5	6	7	8	9	10

$W_s = 1+2+4+6+8 = 21$. H_0 : no treatment effects. H_1 : treatment observations are smaller than control. Reject H_0 if $W_s \leq c$. Find c. Choose c so that $P_{H_0}(W_s \leq c) = 0.05$ (the chance of Type I error is 5%). To determine c, it is necessary to find the null distribution of W_s. $W_s = S_1 + S_2 + \cdots + S_5$ is a distribution like the sum of a sample of size 5 selected from the set $\{1, 2, ..., 10\}$. Each set of 5 treatment ranks has a probability $\frac{1}{\binom{10}{5}} = \frac{1}{252}$. Suppose we want $\alpha = 0.05$. The number x of subsets of $\{1, 2, ..., 10\}$ we must consider is $\frac{x}{252} = 0.05$, or $x = 12.6$. List of treatment ranks and their sum for $n = 5, m = 5$ is

$1+2+3+4+5 = 15$

$1+2+3+4+6 = 16$

$1+2+3+4+7 = 17$

$1+2+3+5+6 = 17$

$1+2+3+4+8 = 18$

$1+2+3+5+7 = 18$

$1+2+4+5+6 = 18$

$1+2+3+4+9 = 19$

$1+2+3+5+8 = 19$

$1+2+3+6+7 = 19$

$1+3+4+5+6 = 19$

$1+2+4+5+7 = 19$

$1+2+3+4+10 = 20$

$1+2+3+5+9 = 20$

$1+2+3+6+8 = 20$

$1+2+4+5+8 = 20$

$1+2+4+6+7 = 20$

$1+3+4+5+7 = 20$

$2+3+4+5+6 = 20$

$W:$	15	16	17	18	19	20	...
$P_{H_0}(W_s = w)$	$\frac{1}{252}$	$\frac{1}{252}$	$\frac{2}{252}$	$\frac{3}{252}$	$\frac{5}{252}$	$\frac{7}{252}$	...

$P_{H_0}(W_s \leq 19) = \frac{12}{252} = 0.0476$. $P_{H_0}(W_s \leq 20) = \frac{19}{252} = 0.0754$. Choose $c = 19$. The actual α is 0.0476. Do not reject H_0.

Properties of the Null Distribution

1. The smallest possible value of W_s is $\frac{n(n+1)}{2}$.
2. $W_{XY} = W_s - \frac{n(n+1)}{2}$ has a symmetric distribution with mean of $E_{H_0}(W_{XY}) = \frac{mn}{2}$. W_{XY} is called the *Mann-Whitney statistic.*
3. Recall that W_R is the sum of the control ranks. $W_r = W_s = 1 + 2 + \cdots + N = \frac{n(n+1)}{2}$.
4. The smallest value W_R can take is $1 + 2 + \cdots + m = \frac{m(m+1)}{2}$.
5. $W_{XY} = W_R - \frac{m(m+1)}{2}$ has a symmetric null distribution with mean $E_{H_0}(W_{XY}) = \frac{mn}{2}$.
6. W_{XY} and W_{YX} have identical null distributions which is tabled, Table B, pages 408-410 in the text book. $P_{H_0}(W_{XY} \leq c | n = k_1, m = k_2) = P_{H_0}(W_{XY} \leq c | n = k_2, m = k_1)$.

We say that X is *stochastically* equal to Y if X and Y have identical distributions. A random variable X has a distribution *symmetric about zero* if $P(X > t) = P(X < -t)$ for all real numbers t.

Example: The Standard Normal Distribution.

Theorem: A random variable x has a distribution symmetric about zero if and only if $X \overbrace{=}^{st} -X$.
proof: The null distribution of W_s is symmetric about $\frac{n(N+1)}{2}$. Rank the observations in inverse order so the observation having rank of 1 now has rank of N, the observation with rank of 2 now has rank of $N-1$, and so on.

Let $S_1', S_2', ..., S_n'$ denote the inverse ranks of the treatment observations. As before, $S_1', S_2', ..., S_n'$ is distributed like a sample of size n selected without replacement from $1, 2, ..., N$. Thus $W_{s'} = S_1' + S_2' + \cdots + S_n'$ has the same null distribution as W_s. But, $S_i' = N - S_i + 1, i = 1, 2, ..., n$. Then, $W_{s'} = S_1' + S_2' + \cdots + S_n' = (N - S_1 + 1) + (N - S_2 + 1) + \cdots + (N - S_n + 1) = n(N+1) = W_s$. Thus, $W_{s'} + W_s = n(N+1)$ or $\left[W_{s'} - \frac{n(N+1)}{2}\right] + \left[W_s - \frac{n(N+1)}{2}\right] = 0$. We have $W_s - \frac{n(N+1)}{2} = -\left[W_{s'} - \frac{n(N+1)}{2}\right] \overbrace{=}^{st} -\left[W_s - \frac{n(N+1)}{2}\right]$.

proof: The null distribution of W_{xy} is symmetric about $\frac{mn}{2}$. $W_{xy} = W_s - \frac{n(N+1)}{2}$, $W_{xy} - \frac{mn}{2} = W_s - \frac{n(n+1)}{2} - \frac{mn}{2} = W_s - \frac{n(N+1)}{2}$. Since $W_s - \frac{n(N+1)}{2}$ has a null distribution symmetric about zero, so does $W_{xy} - \frac{mn}{2}$.

Population Mean and Variance

Under $H_0, W_s = S_1 + S_2 + \cdots + S_n$ is a distribution like a sum of a sample of size n taken without replacement from the finite population $\{1, 2, ..., N\}$. Suppose the population consists of N numbers $v_1, v_2, ..., v_N$. Let v be a random variable denoting one of these numbers selected at random. The probability distribution of v is

$V:$	V_1	V_2	...	V_N
$P(V):$	$\frac{1}{N}$	$\frac{1}{N}$	...	$\frac{1}{N}$

The population mean is $E(V) = \frac{1}{N}\sum_{i=1}^{N} V_i = \bar{V}$. The population variance is $Var(V) = \frac{1}{N}\sum_{i=1}^{n}(V_i - \bar{V})^2 = \tau^2$. Let $T = v_1 + v_2 + \cdots + v_n$ where $(v_1, v_2, ..., v_n)$ is a sample of size n taken without replacement from the population. Note that:

1. Each v_i has the same probability distribution namely $P(V)$.
2. $v_1, v_2, ..., v_n$ are not independent random variables.
3. The pair (v_i, v_j) takes values $(v_k, v_l), l \neq k$ with a probability of $\frac{1}{N(N+1)}$ from $P(A \cap B) + P(A)P(B|A)$.
4. $E(T) = E(v_1 + v_2 + \cdots + v_n) = E(v_1) + E(v_2) = \cdots + E(v_n) = \bar{V} + \bar{V} + \cdots = n\bar{V}$.
5. $Var(T) = E(a_1x_1 + \cdots + a_nx_n) = a_1E(x_1) + \cdots + a_nE(x_n)$. If $x_1, x_2, ..., x_n$ is an iid sequence, then $Var(a_1x_1 + \cdots + a_nx_n) = a_1^2 Var(x_1) + \cdots + a_n^2 Var(x_n)$. If x is not independent then, $Var(T) = \sum_{i=1}^{n} Var(v_i) + \sum_{i \neq j}\sum Cov(v_i, v_j) = \tau^2 + \tau^2 + \cdots + \tau^2 + \sum\sum Cov(v_i, v_j)$.

9.1.2 Tied Observations

Tied observations may occur in two ways:

1. Ordered categories as in the example on page 19 of the text book.
2. With numerical responses as in example on page 21 of the text book.

Example: There are $m = n = 3$, numerical responses. The treatment responses are 4, 9, 9. The control responses are 2, 2, 9. The combined ordered set is 2, 2, 4, 9, 9, 9 and the midranks are 1.5, 1.5, 3, 5, 5, 5.

$S_1^*, S_2^*, ..., S_n^*$ are the midranks of the treatment observations. And, $R_1^*, R_2^*, ..., R_m^*$ are the midranks of the control observations. $W_s^* = S_1^* + S_2^* + \cdots + S_n^*$ is the *midrank sum statistic.* Clearly, W_s^* does not have the same null distribution as before because $(S_1^*, S_2^*, ..., S_n^*)$ does not vary over subsets of $\{1, 2, ..., N\}$.

In the previous example, $W_s^* = 3+5+5 = 13$. Suppose large values of W_s^* indicate the treatment is superior to the control. $\hat{\alpha} = P_{H_0}(W_s^* \geq 13)$. From the set $\{1.5, 1.5, 3, 5, 5, 5\}$ there are 6 choose 3 or 20 equalikely choices under H_0 for each treatment midranks (S_1^*, S_2^*, S_3^*). They are

$1.5 + 1.5 + 3 = 6.$

$1.5 + 1.5 + 5 = 8.$

$1.5 + 1.5 + 5 = 8.$

$1.5 + 1.5 + 5 = 8.$

$1.5 + 3 + 5 = 9.5.$

$1.5 + 3 + 5 = 9.5.$

$1.5 + 3 + 5 = 9.5.$

$1.5 + 3 + 5 = 9.5.$

$1.5 + 3 + 5 = 9.5.$

$1.5 + 3 + 5 = 9.5.$

$3 + 5 + 5 = 13.$

$3 + 5 + 5 = 13.$

$3 + 5 + 5 = 13.$

$5 + 5 + 5 = 15.$

$1.5 + 5 + 5 = 11.5$

$1.5 + 5 + 5 = 11.5$

$1.5 + 5 + 5 = 11.5$

$1.5 + 5 + 5 = 11.5$

$1.5 + 5 + 5 = 11.5$

$1.5 + 5 + 5 = 11.5$

The null distribution is

W	6	8	9.5	11.5	13	15
$P_{H_0}(W_s^* = w)$	$\frac{1}{20}$	$\frac{3}{20}$	$\frac{6}{20}$	$\frac{6}{20}$	$\frac{3}{20}$	$\frac{1}{20}$

$\hat{\alpha} = P_{H_0}(W_s^* \geq 13) = \frac{4}{20}0.20$. Tables of the null distribution of W_s^* are not practical to construct. By the central limit theorem, as $m, n \to \infty$, $\frac{W_s^* - E_{H_0}(W_s^*)}{\sqrt{Var_{H_0}(W_s^*)}} \sim N(0,1)$.

Calculating $E_{H_0}(W_s^*)$ and $Var_{H_0}(W_s^*)$

Let e be the number of distinct values of the combined set $x_1, x_2, ..., x_m$ and $y_1, y_2, ..., y_n$. Let $z_1, z_2, ..., z_e$ denote the distinct ordered values in the combined set. The *ordered* observations in the combined set can be written as:

	# of observations	midrank$= v_i$
z_1	d_1	$\frac{d_1+1}{2}$
z_2	d_2	$d_1 + \frac{d_2+1}{2}$
z_3	d_3	$d_1 + d_2 + \frac{d_3+1}{2}$
.	.	.
.	.	.
.	.	.
z_e	d_e	$d_1 + d_2 + \cdots + \frac{d_e+1}{2}$
	N	

$W_s^* = S_1^* + S_2^* + \cdots + S_n^*$ is the distribution like the total of sample size n taken without replacement from the population

V	v_1	v_2	$\cdots$	v_e
$P_{H_0}(V = v)$	$\frac{d_1}{N}$	$\frac{d_2}{N}$	$\cdots$	$\frac{d_e}{N}$

Let $\bar{v}$ be the population mean. $\bar{v} = \sum_{i=1}^{e} v_i \left(\frac{d_i}{N}\right)$. τ^2 is the population variance. $\tau^2 = \sum_{i=1}^{e}(d_i - \bar{v})\frac{d_i}{N}$. Earlier we showed that $E_{H_0}(W_s^*) = n\bar{v}$, and $Var_{H_0}(W_s^*) = \frac{nm}{N-1}\tau^2$.

$$\bar{v} = \sum_{i=1}^{e} \frac{v_i d_i}{N} = \frac{\left(\frac{d_1+1}{2}\right) d_1 + \left(d_1 + \frac{d_2+1}{2}\right) + \cdots}{N} =$$

$$\frac{\left(\frac{1+2+\cdots+d_1}{d_1}\right)d_1 + \left(\frac{(d_1+1)+(d_1+2)+\cdots+(d_1+d_2)}{d_2}\right)d_2}{N} + \frac{\left(\frac{(d_1+d_2+\cdots+d_{e-1}+1)+\cdots+(d_1+\cdots+d_e)}{d_e}\right)d_e}{N} =$$

$$\frac{1+2+\cdots+N}{N} = \frac{\frac{N(N+1)}{2}}{N} = \frac{N+1}{2} = \bar{v}.$$

Thus, $E_{H_0}(W_s^*) = n\bar{v} = \frac{n(N+1)}{2}$, and

$$\tau^2 = \sum_{i=1}^{e}(v_i - \bar{v})^2 \frac{d_i}{N} = \cdots = \frac{(N+1)(N-1)}{12} - \sum_{i=1}^{e} \frac{d_i(d_i^2-1)}{12N}.$$

So,

$$Var(W_s^*) = \frac{mn(N+1)}{12} - \overbrace{mn\sum_{i=1}^{e}\frac{d_i(d_i^2-1)}{12N(N-1)}}^{\text{Correction for ties}}$$

Example: Page 21 of the text book. 80 boys are randomly divided into a control group of size 40 who receive normal counseling and the treatment group of size 40 who receive special counseling. At the end of the study, each boy is classified as having good, fairly good, fairly poor, or poor adjustment.

Poor	Fairly Poor	Fairly Good	Good	Total	
Treatment:	5	7	16	12	40
Control:	7	9	15	9	40
Total	12	16	31	21	80

Note the ordering of the categories. $d_1 = 12, d_2 = 16, d_3 = 31, d_4 = 21$. The midranks of scores at the lowest category is $\frac{d_1+1}{2} = \frac{12+1}{2} = 6.5$. The midrank of Fairly Poor is $d_1 + \frac{d_2+1}{2} = 12 + \frac{16+1}{2} = 20.5$. The midrank of Fairly Good is $d_1+d_2+\frac{d_3+1}{2} = 44$. The midrank of Good is $d_1+d_2+d_3+\frac{d_4+1}{2} = 70$. H_0 : No treatment effect. H_1 : Treatment effects are larger than the control effects. The test statistic is $W_s^* = \sum$ treatment midranks $=$ $(6.5)5 + (20.5)7 + (44)16 + (70)12 = 1720$. $E_{H_0}(W_s^*) = \frac{n(N+1)}{2} = \frac{40(81)}{2} = 1620$. $Var_{H_0}(W_s^*) = \frac{(40)(40)(81)}{12} - \frac{40(40)}{80(79)}44796$, where $\sum_{i=1}^{4} d_i(d_i^2-1) = 12(12^2-1) + 16(16^2-1) + 31(31^2-1) + 21(21^2-1) = 44796$. Then, $\hat{\alpha} = P_{H_0}(W_s^* \geq 1720) = P_{H_0}\left(\frac{W_s^*-1620}{99.21} \geq \frac{1720-1620}{99.21}\right) = P(z \geq 1.01) = .16$. Problem 42 in Chapter 1 of the text book is similar. Problem 46, Chapter 1, has a tie.

9.1.3 Relationship of W_s^* to the Mann-Whitney Statistic

When ties are present, the Mann-Whitney statistic is calculated as $W_{xy}^* = [\#\ \text{pairs}(x_i, y_j) \text{ with } x_i < y_i]$ $+\frac{1}{2}[\#\ \text{pairs}(x_i, y_j) \text{ with } x_i = y_j]$. On page 22 of the text book, it is shown that $W_{xy}^* = W_s^* - \frac{n(n+1)}{2}$. $E_{H_0}(W_{xy}^*) = E_{H_0}(W_s^*) - \frac{n(n+1)}{2} = \frac{n(N+1)}{2} - \frac{n(n+1)}{2} = \frac{mn}{2}$.

9.1.4 Two Sided Alternative

Example: This is Example 4 on page 27 of the text book. 16 subjects are randomly divided into a group of 8 to be hypnotized and a group of 8 controls. Measures of each subject's ventilation were obtained. H_0 : No treatment effects. H_1 : Treated group has lower scores or higher scores than the control group.

Control:	3.99	4.19	4.21	4.54	4.64	4.69	4.84	5.48
Treatment:	4.36	4.67	4.78	5.08	5.16	5.20	5.52	5.74

$n = m = 8$. $\alpha = 0.05$. The test statistic is $W_s = 87$. $E_{H_0}(W_S) = \frac{n(N+1)}{2} = \frac{8(17)}{2} = 68$. The distribution of W_s is symmetric about 68. So, reject H_0 if $W_s \leq 68 - c$ or if $W_s \geq 68 + c$. Find c so that $P_{H_0}(W_s \leq 68 - c$ or $W_s \geq 68 + c) = 0.05$, $P_{H_0}(W_s \leq 68 - c) = P_{H_0}(W_s \geq 68 + c) = 0.025$. Using Table B in the text book, $W_{xy} = W_s - \frac{n(n+1)}{2} = W_s - \frac{8(9)}{2} = 36$. $0.025 = P_{H_0}(W_s - 36 \leq 68 - c - 36) = 0.025 - P_{H_0}(W_{xy} \leq 32 - c)$. From Table B, $P(W_{xy} \leq 13) = 0.0249$. Then, $32 - c = 13 \Rightarrow c = 19$. Reject H_0 if $|W_s - 68| \geq c = 19$. Since $|87 - 68| = 19 \Rightarrow$ Reject H_0 The p-value is $2P_{H_0}(W_s \geq 87) = 2P_{H_0}(W_{xy} \geq 87 - 36) = 2P_{H_0}(W_{xy} \geq 51) = 1 - 2P_{H_0}(W_{xy} \leq 50) = 1 - 2(0.0249) = 0.0498$.

9.2 Siegel-Tukey and Smirnov Tests

The rank sum test assumes that the effect of a treatment, if any, is to increase or decrease the response. We now show that a similar statistic based on dispersion ranks can be used to test the hypothesis of equal variances. The Siegel-Tukey tests H_0 : No differences in variance, H_1 : Treatment response is less variable than the control response. If H_1 is true, then the largest and smallest observations are likely to be control observations. this suggests assigning low ranks to the extremes and have the ranks increase toward the center. One scheme for assigning ranks is as follows:

1. Form a combined ordered set.
2. Assign rank 1 to the smallest, rank 2 to the largest, rank 3 to the second largest, rank 4 to the second smallest, etc.

If the treatment observations are less variable, then they will tend to be in the center of this set and their sum will tend to be large. The null distribution of W_s(equal to the dispersion ranks) is the same as for the rank sum test. Note: Table B in the text book can be used to determine the critical value. A normal approximation can be used if m, n are large. If ties are present, then use the correction for ties method.

Example:

Treatment:	0.26	0.31	0.38	0.40	0.55	0.64
Control:	0.10	0.14	0.34	0.60	0.80	

$m = 5, n = 6$. The combined set is 0.10, 0.14, 0.26, 0.31, 0.34, 0.38, 0.40, 0.55, 0.60, 0.64, 0.80. The dispersion ranks are 1, 4, 5, 8, 9, 11, 10, 7, 6, 3, 2. The test statistic is $W_s = 5 + 8 + 11 + 10 + 7 + 3 = 44$. Reject H_0 if $W_s \geq c$. $\hat{\alpha} = P_{H_0}(W_s \geq 44)$. $W_{xy} = W_s - \frac{6(7)}{2} = W_s - 21 \Rightarrow P_{H_0}(W_{xy} \geq 44 - 21) = P_{H_0}(W_{xy} \geq 23)$. $E_{H_0}(W_{xy}) = \frac{mn}{2} = 15$. $P_{H_0}(W_{xy} \leq 7) = 0.089$.

1. The Siegel-Tukey test assumes that the control and the treatment observations are centered at the same value.
2. The Siegel-Tukey test lacks symmetry. Another test with the same properties is obtained by reversing the ranks. Typically, both procedures lead to the same conclusion, but not always the same p-value.

9.2.1 The Smirnov Test

The Kolmogorov-Smirnov statistical test tests for the equality of two sample distributions from the same population. Results show that the Kolmogorov-Smirnov test does not have much statistical power for either parameter, separately. When this test rejects the null hypothesis that the two distributions are the equal, then further analyzes are needed to determine if the scale parameter or the location parameter, or both are statistically different.

The test is based on comparing the sample cumulative distribution functions determined from two independent samples. Notation: $x_1, x_2, ..., x_m$ is a sample of m observations from a population with cdf $F(t)$.

$F_m(t)$ is the sample cdf of the x's which is equal to $\frac{\#(X_i \leq t)}{m}, -\infty < t < \infty$. $y_1, y_2, ..., y_n$ is a sample of n observations from a population with cdf $G(t)$. $G_n(t)$ is equal to the sample cdf of the y's which is equal to $\frac{\#(y_i \leq t)}{n}, -\infty < t < \infty$. The Smirnov statistic is $D_{mn} = max_t|G_n(t) - F_m(t)|$. The hypotheses are, $H_0 : F(t) = G(t), \forall t$ versus $H_1 : F(t) \neq G(t)$, for some t. Reject H_0 if $D_{mn} \geq c$. Note that $F_m(t)$ and $G_n(t)$ are non decreasing step functions with smallest and largest values being 0 and 1. They are also right continuous.

Example: Calculate the Smirnov statistic.

Control(X)	3.1	4.2	4.9	6.8	F_m
Treatment(Y)	0.0	2.1	2.8	4.4	G_n

Notation: Let $x_{(1)} < z_{(2)} < \cdots < z_{(N)}$, where $N = n + m$ denote the combined ordered set of values. The combined order set is

Combined Set:	$\underline{0.0}$	$\underline{2.1}$	$\underline{2.8}$	3.1	$\underline{4.2}$	4.4	4.9	6.8
Rank:	1	2	3	4	5	6	7	8
$4G_n = \#(Y's \leq z_{(i)})$:	1	2	3	3	3	4	4	4
$4F_m = \#(X's \leq z_{(i)})$:	0	0	0	1	2	2	3	4

The max difference is $D_{mn} = |\frac{3}{4} - \frac{0}{4}| = \frac{3}{4}$. Since the maximum value occurs at a point in the combined ordered set, it is not necessary to graph $F_m(t)$ and $G_n(t)$ to calculate the Smirnov statistic. Under H_0, each ordering of the $X's$ and $Y's$ is equally likely. There are $\begin{pmatrix} N \\ n \end{pmatrix}$. ways(positions for the $Y's$) to order the $X's$ and the $Y's$. In our example, there are $\begin{pmatrix} 8 \\ 4 \end{pmatrix} = 70$ distinct orderings of the $X's$ and the $Y's$. To get the null distribution, we would have to list all of these and in each case calculate D_{mn}.

9.2.2 Tabulated Null Distribution

1. Table E in the text book gives $P_{H_0}(D_{mn} \geq d)$ for $n = m = 1, 2, ..., 30$.

2. $\lim_{n,m\to\infty} P\left(\sqrt{\frac{mn}{m+n}} D_{mn} \geq z\right)$ where $k(z) = 1 - 2\sum_{k=1}^{\infty}(-1)^k \exp^{-2k^2z^2}, z \geq 0$ is the limiting distribution. The limiting distribution is not Normal because D_{mn} cannot be expressed as a sum of independent random variables as is required to invoke the Central Limit Theorem.

3. $k(z)$ is given in Table F of the text book.

4. The distribution of $\sqrt{\frac{mn}{m+n}} D_{mn}$ converges slowly to $k(z)$. Table F gives an adequate approximation only if $m = n \geq 30$.

5. Our text does not give tables for the case when $m \neq n$. Such tables are available but an extensive table is required.

6. In the presence of ties, the null distribution of D^*_{mn} is not in Tables E or F. But, $P_{H_0}(D^*_{mn} \geq d) \leq P_{H_0}(D_{mn} \geq d)$.

9.3 Homework and Answers

Chapter 1 homework.

17: Find $P_H(W_s \leq w)$. (i) $m = 5, n = 6. \Rightarrow k_1 = 5, k_2 = 6. \frac{n(n+1)}{2} = \frac{6(7)}{2} = 21$. $w = 21$. $P(W_s \leq 21) = P(w_s \leq 21 - 21) = P(W_{XY} \leq 0) = 0.0022$. (ii) $w = 23, m = 6, n = 4$. $\frac{n(n+1)}{2} = \frac{4(5)}{2} = 10$. $P(W_s \leq 23 = P(W_{XY} \leq 13) = 0.6190$. (iii) $m = n = 7$. $w = 34$. $\frac{n(n+1)}{2} = \frac{7(8)}{2} = 28$. $P(W_s \leq 34) = P(W_{XY} \leq 6) = 0.0087$.

25: The data are:

Controls: 20	21	24	30	32	36	40	48	54
Treatments: 19	22	25	26	28	29	34	37	38

The rank ordered set is: 19(1), 20(2), 21(3), 22(4), 24(5), 25(6), 26(7), 28(8), 29(9), 30(10), 32(11), 34(12), 36(13), 37(14), 38(15), 40(16), 48(17), 54(18). $m = n = 9$. $W_s = 76$. $\frac{9(10)}{2} = 45$. $P(W_{XY} \leq 76 - 45) = P(W_{XY} \leq 31) = 0.2181$.

37(i): Find the Normal approximation to the probability $P_H(W_s \geq w)$ both with and without continuity correction, and compare it with the value given in Table B, when $m = 5, n = 3$ and (i) $w = 9$, (ii) $w = 11$, and (iii) $w = 13$.

(i) $E_{H_0}(W_s) = \frac{n(N+1)}{2} = \frac{3(9)}{2} = 13.5$. $\sqrt{Var_{H_0}(W_s)} = \sqrt{\frac{mn(N+1)}{12}} = \sqrt{\frac{5(3)(9)}{12}} = \sqrt{11.25} = 3.35$. Table B gives $W_{xy} = W_s - \frac{n(n+1)}{2} = W_s - 6$. $P_{H_0}(W_s \geq 9) = 1 - P_{H_0}(W_s \leq 8) = 1 - P_{H_0}(W_{xy} \leq 2) = 1 - 0.0714 = 0.9286$. The normal approximation without continuity correction is $P(W_s \geq 9) = P\left(\frac{W_s - 13.5}{3.35} \geq \frac{9 - 13.5}{3.35}\right) = 1 - \Phi(-1.34) = \Phi(1.34) = 0.9099$. The normal approximation with continuity correction is $P(W_s \geq 8.5) = P\left(\frac{W_s - 13.5}{3.35} \geq \frac{8.5 - 13.5}{3.35}\right) = 1 - \Phi(-1.49) = \Phi(1.49) = 0.9319$.

38(i): The ordered set is –6(1), –5(2), 0(3), 1(4), 2(5), 4(6), 5(7), 6(8), 9(9), 16(10). $W_s = 1+2+4+6+8 = 21$. $W_{XY} = W_s - \frac{n(n+1)}{2} = W_s - 15$. $E_{H_0}(W_s) = \frac{n(N+1)}{2} = 27.5$ $Var_{H_0}(W_s) = \frac{mn(N+1)}{2} = 137.5$. $P_{H_0}(W_s \leq 21) = P(W_s \leq 21.5) = P_{H_0}\left(\frac{W_s - 27.5}{11.73} \leq \frac{21 - 27.5}{11.73}\right) = \Phi(-0.5541) = 0.2912$.

39(iii): In the situation of Problem 23, use the normal approximation to determine for what values of W_s to reject the hypothesis of no difference at significance level $\alpha = 0.05$ when (i) $m = 20, n = 15$; (ii) $m = 15, n = 20$; (iii) $m = n = 25$; (iv) $m = 20, n = 30$. Here n is the number of guinea pigs receiving the orange juice. The data from Problem 23 is

Controls:	20	21	24	30	32	36	40	48	54
Treatment:	19	22	25	26	28	29	34	37	38

(iii) Reject H_0 if $W_s \geq c$. Use the normal approximation to determine c, when $\alpha = 0.05$. $E_{H_0}(W_s) = \frac{n(N+1)}{2} = \frac{25(51)}{2} = 637.5$. $\sqrt{Var_{H_0}(W_s)} = \sqrt{\frac{mn(N+1)}{12}} = \sqrt{\frac{25(25)(51)}{12}} = 51.54$. We want $0.05 = P(W_s \geq c - 0.5) = P\left(z > \frac{c - 0.5 - 637.5}{51.54}\right)$. So, $\frac{c - 638}{51.54} = 1.645$. Thus, $c = 722.8$. Round up to $c = 723$.

43 Let the treatment and control observations be –3, –3, 0, 1 and –3, 1, 2, 2, respectively. Find the significance probability if small values of W_s^* are significant. The combined set is –3, –3, –3, 0, 1, 1, 2, 2. $m = n = 4$. The midranks are 2, 2, 2, 4, 5.5, 5.5, 7.5, 7.5. W_s^* is the sum of the midranks for the treatments. $W_s^* = 13.5$. The significance probability is $P_{H_0}(W_s^* \leq 13.5)$. m, n are not large enough to use the normal approximation. There are $e = 4$ distinct values and $d_1 = 3, d_2 = 1, d_3 = 2, d_4 = 2$. There are $\binom{8}{4}$ equally likely ways of choosing a subset of 4 of the midranks from the population $\{2, 2, 2, 4, 5.5, 5.5, 7.5, 7.5\}$.

S_1^*	S_2^*	S_3^*	S_4^*	W_s^*	Probability
2	2	2	4	10	$\frac{1}{70}$
2	2	2	5.5	11.5	$\frac{1}{70}$
2	2	2	5.5	11.5	$\frac{1}{70}$
2	2	4	5.5	13.5	$\frac{1}{70}$
2	2	4	5.5	13.5	$\frac{1}{70}$
2	2	4	5.5	13.5	$\frac{1}{70}$
2	2	4	5.5	13.5	$\frac{1}{70}$
2	2	4	5.5	13.5	$\frac{1}{70}$
2	2	4	5.5	13.5	$\frac{1}{70}$
2	2	4	7.5	13.5	$\frac{1}{70}$
2	2	4	7.5	13.5	$\frac{1}{70}$

$P_{H_0}(W_s) \leq 13.5) = \frac{11}{70}$.

51(i):

60: Treatment: 1.5, 1.8, 1.9, 2.3, 2.5, 2.8; $n = 6$. Control: 0.8, 1.4, 2.1, 2.7, 3.1; $m = 5$. H_0 : No difference in dispersion for treatment and control. H_1 : the treatment responses have smaller dispersion than the control responses. Determine the significance probability for the Siegel-Tukey test if: (i) ranking is as in Figure 1.6 of the text book, (ii) ranking is the mirror image of Figure 1.6.

Solution to (i): The combined set and dispersion ranks are 0.8(1), 1.4(4), 1.5(5), 1.8(8), 1.9(9), 2.1(11), 2.3(10), 2.5(7), 2.7(6), 2.8(3), 3.1(2). W_s = sum of the treatment dispersion ranks $= 5+8+9+10+7+3 = 42$. Reject H_0 if $W_s \geq c$. $\hat{\alpha} = P_{H_0}(W_s \geq 42) = P_{H_0}(W_s - 21 \geq 42 - 21) = P_{H_0}(W_{XY} \geq 21)$. $E_{H_0}(W_{XY}) = \frac{mn}{2} = \frac{5(6)}{2} = 15$. Thus, $\hat{\alpha} = P_{H_0}(W_{XY} \leq 9) = 0.1645$ from Table B in the text book.

Solution to (ii): The combined set and dispersion ranks are: 0.8(2), 1.4(3), 1.5(6), 1.8(7), 1.9(10), 2.1(11), 2.3(9), 2.5(8), 2.7(5), 2.8(4), 3.1(1). W_s = sum of the treatment dispersion ranks $= 6 + 7 + 109 + 8 + 4 = 44$. Reject H_0 if $W_s \geq c$. $\hat{\alpha} = P_{H_0}(W_s \geq 44)$. $W_{XY} = W_s - \frac{n(n+1)}{2} = W_s - 21$. $E_{H_0}(W_{XY}) = \frac{mn}{2} = 15$. $P_{H_0}(W_{XY} \geq 23) = P_{H_0}(W_{XY} \leq 7) = 0.0887$ from Table B in the text book.

65: $H_0 : F = G$ $H_1 : F \neq G$. In problem 64, $m = n = 9$. $\hat{\alpha} = P_{H_0}\left(D_{mn} \geq \frac{3}{9}\right)$. We can determine $\hat{\alpha}$ from Table E in the text book since $m = n = 9$. From Table E, $\hat{\alpha} = 0.7301$. In problem 25, we used the rank sum test to test the hypotheses $H_0 : F = G$. $H_1 : Y$'s tend to be smaller than the X's. We found the significance probability, for a one-tailed test to be $\hat{\alpha} = 0.2181$. This significance probability is smaller than when using the Smirnov test because: (1) it is a one-tailed test, and (2) the rank sum test is better(more powerful) for detecting specific types of departures from H_0.

66(i): Determine the null distribution of D_{mn} if (i) $m = 3, n = 2$; (ii) $m = 3, n = 4$. The number of cases is $\binom{5}{2} = 10$.

	X	X	X	Y	Y
$3F_m$	1	2	3	3	3
$2G_n$	0	0	0	1	2

$D_{mn} = 1$.

	X	X	Y	X	Y
$3F_m$	1	2	2	3	3
$2G_n$	0	0	1	1	2

$D_{mn} = \frac{2}{3}$.

	X	Y	X	X	Y
$3F_m$	1	1	2	3	3
$2G_n$	0	1	1	1	2

$D_{mn} = \frac{1}{2}$.

	Y	X	X	X	Y
$3F_m$	0	1	2	3	3
$2G_n$	1	1	1	1	2

$D_{mn} = \frac{1}{2}$.

	X	X	Y	Y	X
$3F_m$	1	2	2	2	3
$2G_n$	0	0	1	2	2

$D_{mn} = \frac{2}{3}$.

	X	Y	X	Y	X
$3F_m$	1	1	2	2	3
$2G_n$	0	1	1	2	2

$D_{mn} = \frac{1}{3}$.

	Y	X	X	Y	X
$3F_m$	0	1	2	2	3
$2G_n$	1	1	1	2	2

$D_{mn} = \frac{1}{2}$.

	X	Y	Y	X	X
$3F_m$	1	1	1	2	3
$2G_n$	0	1	2	2	2

$D_{mn} = \frac{2}{3}$.

	Y	X	Y	X	X
$3F_m$	0	1	1	2	3
$2G_n$	1	1	2	2	2

$D_{mn} = \frac{2}{3}$.

	Y	Y	X	X	X
$3F_m$	0	0	1	2	3
$2G_n$	1	2	2	2	2

$D_{mn} = 1$. $D_{mn} = \max_t |F_m(t) - G_n(t)|$. The null distribution is

Z	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{2}{3}$	1
$P_{H_0}(D_{mn} = z)$	$\frac{1}{10}$	$\frac{3}{10}$	$\frac{4}{10}$	$\frac{2}{10}$

9.4 Variance of W_{xy} when $m = n = 2$

We shall need the following general result concerning variance: Let $u_1, u_2, ..., u_n$ be any random variables and let $T = u_1 + u_2 + \cdots + u_n$. Then, $Var(T) = \sum_{i=1}^{n} Var(u_i) + 2\sum_{i<j} Cov(u_i, u_j)$. We will apply this to $W_{xy} = \sum_{i=1}^{m}\sum_{j=1}^{n} \Phi(x_i, y_j)$. Consider the case $m = n = 2$. Then, $W_{xy} = \Phi(x_1, y_1) + \Phi(x_1, y_2) + \Phi(x_2, y_1) + \Phi(x_2, y_2)$ where

$$\Phi(x, y) = \begin{cases} 1, & \text{if } x < y \\ 0, & \text{otherwise} \end{cases}$$

Let $u_{ij} = \Phi(x_i, y_j), i, j = 1, 2$. Then, $W_{xy} = u_{11} + u_{12} + u_{21} + u_{22}$. To calculate the variance of W_{xy}, we need to determine $Var(u_{ij})$ and the covariances of all pairs. The u_{ij}'s are binary random variables that take only the values 0 and 1. $P(u_{ij} = 1) = P(x_i < y_j) = p_1$. $P(u_{ij} = 0) = 1 - p_1$. Thus, the probability distribution of u_{ij} is

u	0	1
$P(u_{ij} = u)$	$1 - p_1$	p_1

$E(u_{ij}) = 0(1 - p_1) + 1p_1 = p_1$. $Var(u_{ij}) = E(u_{ij}^2) - [E(u_{ij})]^2 = p_1 - p_1^2$. $Cov(u_{11}, u_{12}) = E(u_{11}u_{12}) - E(u_{11})E(u_{12})$. We have already determined that $E(u_{11}) = E(u_{12}) = p_1$. To determine $E(u_{11}u_{12})$ note that the product is a binary random variable that can take only the values 0 and 1. Thus, $E(u_{11}, u_{12}) = 0P(u_{11}u_{12} = 0) + 1P(u_{11}u_{12} = 1) = P(u_{11} = 1 \text{ and } u_{12} = 1) = P(x_1 < y_1 \text{ and } x_1 < y_2) = p_2$(by definition of p_2. We have $Cov(u_{11}, u_{12}) = E(u_{11}u_{12}) - E(u_{11})E(u_{12}) = p_2 - p_1^2$. $Cov(u_{11}, u_{21}) = E(u_{11}u_{21}) - E(u_{11}E(u_{21})$. As before, $E(u_{11}u_{21}) = P(u_{11}u_{21} = 1) = P(x_1 < y_1 \text{ and } x_2 < y_1) = p_3$. Thus, $Cov(u_{11}, u_{21}) = E(u_{11}u_{21}) - E(u_{11})E(u_{21}) = p_3 - p_1^2$. Note u_{11} is a function of (x_1, y_1) only. u_{22} is a function of (x_2, y_2). Since (x_1, y_1) and (x_2, y_2) are independent, it follows that u_{11} and u_{22} are independent. Thus $Cov(u_{11}, u_{22}) = 0$. $Cov(u_{12}, u21) = E(u_{12}u_{21}) - E(u_{12})E(u_{21})$. As before, $E(u_{12}) = E(u_{21}) = p_1$. u_{12} is a function of (x_1, y_2). u_{21} is a function of (x_2, y_1). By independence, $Cov(u_{11}, u_{21}) = 0$. $Cov(u_{12}, u_{22}) = E(u_{12}u_{22}) - E(u_{12})E(u_{22})$. As before, $E(u_{12}) = E(u_{22}) = p_1$. $E(u_{12}u_{22}) = P(u_{12}u_{22} = 1) = P(x_1 < y_2 \text{ and } x_2 < y_2) = p_3$(by definition of p_3). Thus, $Cov(u_{12}, u_{22}) = p_3 - p_1^2$. $Cov(u_{21}, u_{22}) = E(u_{21}u_{22}) - E(u_{21})E(u_{22})$. As before, $E(u_{21}) = E(u_{22}) = p_1$. $E(u_{21}u_{22}) = P(u_{21}u_{22} = 1) = P(x_2 < y_1 \text{ and } x_2 < y_2) = p_2$(by definition of p_2). Thus, $Cov(u_{21}, u_{22}) = p_2 - p_1^2$. Then, we have $Var(W_{xy}) = Var(u_{11}) + Var(u_{12}) + Var(u_{21}) + Var(u_{22}) + 2Cov(u_{11}, u_{12}) + 2Cov(u_{11}, u_{21}) + 2Cov(u_{11}, u_{22}) + 2Cov(u_{12}, u_{21}) + 2Cov(u_{12}, u_{22}) + 2Cov(u_{21}, u_{22}) = 4p_1(1 - p_1) + 2(p_2 - p_1^2) + 2(p_3 - p_1^2) + 0 + 0 + 2(p_3 - p_1^2) + 2(p_2 - p_1^2) = 4p_1(1 - p_1) + 4(p_2 - p_1^2) + 4(p_3 - p_1^2)$.

9.5 Population Models

The randomization model does not provide a basis for studying the power of a test(ie the probability of rejecting H_0 when H_1 is true). In addition, the randomization model does not provide a basis for sample size determination. In Chapter 2 of the text book, we introduce several population models and study the following problems:

1. Power of the rank sum test(section 2).
2. Asymptotic power and sample size determination(section 3).
3. Estimating the shift parameter(section 5).
4. Confidence limits for the shift parameter(section 6).

The rank sum test applies to the following situations:

Model 2 Comparison of two treatments. N subjects are drawn in a simple random sample from a single population of potential users of the treatments. The N subjects are randomly assigned, m to one treatment and n to the other treatment.

Model 3 Comparison of two attributes or subpopulations. Random samples of sizes m and n are drawn from each of the two populations.

Model 4 Comparison of two attributes or subpopulations. A single sample of size N is selected from a population where m of them belong to one population and n of them to another.

The assumptions are that the populations are sufficiently large so that $x_1, x_2, ..., x_m$ and $y_1, y_2, ..., y_n$ are independent random samples. For models 2-4 $x_1, x_2, ..., x_m$ are iid with cdf $F(t)$. $y_1, y_2, ..., y_n$ are iid with cdf $G(t)$. For model 4, the sets are conditionally iid given m, n. The null hypothesis of no treatment effect is $H_0 : F = G$. Under H_0, the combined set $x_1, x_2, ..., x_m, y_1, y_2, ..., y_n$ of random variables are iid with common cdf say $F(t)$.

Theorem: If $F(t)$ is continuous, then under H_0, the ranks of $y_1, y_2, ..., y_n$ in the combined ranking have the null distribution studied in previous sections. That is $P_{H_0}(S_1 = s_1, ..., S_n = s_n) = \frac{1}{\binom{N}{n}}$. That is, the null distribution does not depend on F so all rank statistics are distribution free. proof: Let $z_1, z_2, ..., z_N$ denote the combined set where $N = m + n$. There are $N!$ orderings of $z_1, z_2, ..., z_N$. Each ordering has the same probability. Ties occur with probability zero since the distribution is continuous. $P_{H_0}(S_1 = s_1, ..., S_n = s_n) = \frac{(\text{\# ways of permuting n x's})(\text{\# ways of permuting m y's})}{N!} = \frac{n!m!}{N!} = \frac{1}{\binom{N}{n}}$.

9.5.1 Null Distribution of W_s^* when F is Discrete

If F is not continuous, then ties can occur with positive probability and the midranks are not distribution free.

Example: Let F be discrete with the following pdf,

x	a	b
$f(x)$	p	q

Consider the case $m = 2$ and $n = 1$. Under H_0 x_1, x_2, y_1 are iid with the above pdf. S_1^* is the midrank of y_1 in the combined set. e is the number of distinct values of x_1, x_2, y_1. d_1 is the number of observations tied at the smallest value. d_2 is the number of observations tied at the next smallest value.

x_1	x_2	y_1	Probability	S_1^*	e, d_1, d_2
a	a	a	p^3 2	1,3,0	
a	a	b	p^2q	3	2,2,1
a	b	a	p^2q	1.5	2,2,1
b	a	a	p^2q	1.5	2,2,1
b	b	a	pq^2	1	2,1,2
b	a	b	pq^2	2.5	2,1,2
a	b	b	pq^2	2.5	2,1,2
b	b	b	q^3	2	1,3,0

The distribution of S_1^* depends on F.

s	1	1.5	2	2.5	3
$P_{H_0}(S_1^* = s)$	pq^2	$2p^2q$	$p^3 + q^3$	$2pq^2$	p^2q

Suppose in the previous example that we are to reject H_0 if $W_s^* \geq c$ where $W_s^* = S_1^*$. Suppose the observed value of W_s^* is $W_s^* = 3$. Then, the observed significance level is $\hat{\alpha} = P_{H_0}(W_s^* \geq 3) = p^2q$. Thus $\hat{\alpha}$ cannot be computed if the values of p and q are unknown. (e, d_1, d_2) is called the *tie configuration.* Calculation of the observed significance level conditional on the observed tie configuration: Suppose we observe $W_s^* = 3$ and the tie configuration is $(2, 2, 1)$. Then, the conditional p-value is $P_{H_0}(W_s^* \geq 3|(2,2,1)) = \frac{p^2q}{p^2q+p^2q+p^2q} = \frac{p^2q}{3p^2q} = \frac{1}{3}$. The conclusion is that the conditional distribution of the midranks given the tie configuration is distribution free but is not valid for the entire population. This difficulty diminishes as m, n increase since both the conditional and unconditional distributions of $\frac{W_s^* - E_{H_0}(W_s^*)}{\sqrt{Var_{H_0}(W_s^*)}}$ have a limiting normal distribution.

9.5.2 Power of the Rank Sum Test

The *power of a test* is the probability of rejecting H_0 given that some particular alternative to H_0 is true. In general, $H_1 : F \neq G$ describes all possible alternatives to H_0. However, we are mainly interested in alternatives where the new treatment is more or less effective than the standard treatment. Recall that x is the response of a control subject and y is the response of a treatment subject. We say that Y is *stochastically larger* than X if $P(Y > t) \geq P(X > t), \forall -\infty < t < \infty$.

Example: Let X, Y be independent and have exponential distributions.

$$F(t) = P(X \leq t) = \begin{cases} 1 - e^{-\alpha t}, & t \geq 0 \\ 0, & t < 0 \end{cases}$$

$$G(t) = P(Y \leq t) = \begin{cases} 1 - e^{-\beta t}, & t \geq 0 \\ 0, & t < 0 \end{cases}$$

where α, β are parameters such that $\alpha > 0$ and $\beta > 0$. $E(x) = \frac{1}{\alpha}$ and $E(y) = \frac{1}{\beta}$. Under what conditions on α, β is it true that $\overbrace{Y \geq X}^{\text{st}}$? Solution: $P(Y > t) = 1 - G(t) = e^{-\beta t}$ if $t \geq 0$. $P(X > t) = 1 - F(t) = e^{-\beta t}$ if $t \geq 0$. Then, $P(Y > t) \geq P(X > t), \forall t$ iff $e^{-\beta t} \geq e^{-\alpha t} \forall t > 0$ iff $\beta \leq \alpha$. A special case of stochastically ordered random variables is described by the shift model. A pair of independent random variables X and Y follow the *shift model* if $Y \overbrace{=}^{\text{st}} X + \Delta$ where Δ is a constant such that $-\infty < \Delta < \infty$. Under the shift model, $E(y) = E(x + \Delta) = E(x) + \Delta$ so that $\Delta = E(y) - E(x)$ which is the *mean difference.* We cannot describe the shift model by the statement $Y = X + \Delta$ because then it is not possible for X and Y to be independent random variables. If $Y \overbrace{=}^{\text{st}} X + \Delta$ then $G(t) = P(Y \le t) = P(X + \Delta \le t) = P(X \le t - \Delta) = F(t - \Delta)$. Thus, and equivalent way to specify the shift model is that $G(t) = F(t - \Delta)\forall t$. The interpretation of the shift model is (1) $\Delta > 0$ means that the treatment increases the response, (2) $\Delta = 0$ means $F = G$ and (3) $\Delta < 0$ means that the treatment decreases the response.

9.5.3 Power of the Wilcoxon Test

Recall that $W_{XY} = W_s - \frac{n(n+1)}{2}$ and W_{XY} is the number of pairs (X_i, Y_j) for which $X_i < Y_j$. We now study the power of the Wilcoxon test under the shift model $Y \overbrace{=}^{\text{ST}} X + \Delta$ where X has a continuous cdf $F(t)$. $H_0 : \Delta = 0$, no treatment effects. $H_1 : \Delta > 0$ treatment tends to increase the response. Reject H_0 if $W_{XY} \ge c$. The definition of the *power function* is $\prod_F(\Delta) = P_\Delta(W_{XY} \ge c)$. Notes:

1. $P_\Delta(W_{XY} \ge c)$ is the probability of rejecting the null hypothesis given the true value of the shift parameter is Δ.

2. $\prod_F(0) = P_o(W_{XY} \ge c) = P_{H_0}(W_{XY} \ge c)$ where the critical value c is chosen so that the significance level is some prescribed value, say α. That is, $\prod_F(0) = \alpha$.

Theorem(main result of Section 2 in the text book): Under the shift model, $\prod_F(\Delta)$ is a non-decreasing function of Δ, $-\infty < \Delta < \infty$. Proof: Let $\Delta_0 < \delta_1$. We will show that $\prod_F(\Delta_0) \le \prod_F(\Delta_1)$. Let $x_1, x_2, ..., x_m$ be iid with cdf F, and let $u_1, u_2, ..., u_n$ be iid with cdf F. If Δ_0 is the true value of Δ then $Y_j \overbrace{=}^{\text{ST}} u_j + \Delta_0$. If Δ_1 is the true value of Δ, then the $Y's$ are distributed like $Y_j' \overbrace{=}^{\text{ST}} u_j + \Delta_1$. How are the Y_j and Y_j' related? Answer: $Y_j' \overbrace{=}^{\text{ST}} u_j + \Delta_1 = (u_j + \Delta_0) + (\Delta_1 - \Delta_0) \overbrace{=}^{\text{ST}} Y_j + (\Delta_1 - \Delta_0)$. Let W_{XY} be the number of pairs (x_i, y_j) for which $x_i < y_j$ and $W_{XY'}$ be the number of pairs (x_i, y_j') for which $x_i < y_j'$. How are W_{XY} and $W_{XY'}$ related? Answer: $W_{XY'}$ is the number of pairs (x_i, y_j') for which $x_i < y_j'$ which is equal to the number of pairs (x_i, y_j) for which $x_i < y_j + (\Delta_1 - \Delta_0)$ where we have replaced y_j' by $y_j + (\Delta_1 - \Delta_0)$. Thus(keep in mind that $\Delta_1 > \Delta_0$) $W_{XY'}$ is equal to the number of pairs (x_i, y_j) for which $x_i - y_j < \Delta_1 - \Delta_0$ which is equal to the number of pairs (x_i, y_j) for which $x_i - y_j < 0$ plus the number of pairs (x_i, y_j) for which $0 \le x_i - y_j < \Delta_1 - \Delta_0$ which is equal to $W_{XY} + v$ where v is a non-negative random variable. Thus, $W_{XY} \overbrace{=}^{\text{ST}} W_{XY'}$ and $\prod_F(\Delta_0) = P_{\Delta_0}(W_{XY} \ge c) \le P_{\Delta_1}(W_{XY'} \ge c) = \prod_f(\Delta_1)$. Implications of the theorem are:

1. If $\Delta > 0$ then $\prod_f(\Delta) \ge \prod_F(0) = \alpha$. A test whose power against a class of alternatives never falls below the α level is said to be *unbiased* against that class of alternatives. Thus, we have shown that the on-tailed Wilcoxon test is unbiased against one-sided shift alternatives.

2. $\prod_f(\Delta) \le \alpha$ for $\Delta < 0$. This property guarantees that the probability of adopting the new treatment when it is actually worse than the standard one never exceeds α.

3. An α level test of $H_0 : \Delta = 0$ versus $H_1 : \Delta > 0$ is also an α level test of $H_0 : \Delta \le 0$ versus $H_1 : \Delta > 0$. Reason: $\prod_F(\Delta) \le \alpha$ for $\Delta \le 0$ so the Type I error probability never exceeds α.

9.5.4 Asymptotic Power

We assume F, G are continuous(i.e. no ties). We study the power of the rank sum test by using the Mann Whitney statistic, W_{XY} which is the number of pairs (x_i, y_j) for which $x_i < y_j$ which is equal to $\sum_{i=1}^m \sum_{j=1}^n \Phi(x_i, y_j)$ where

$$\Phi(x, y) = \begin{cases} 1, & x < y. \\ 0, & \text{otherwise.} \end{cases}$$

As $m, n \to \infty$, the distribution of $\frac{W_{XY}-E(W_{XY})}{\sqrt{Var(W_{XY})}}$ converges to the standard normal.

Theorem: Let $x_1, x_2, ..., x_m$ be iid with cdf F. Let $y_1, y_2, ..., y_n$ be iid with cdf G. Then, $E(W_{XY}) = mnp_1$ and $Var(W_{XY}) = mnp_1(1-p_1) + mn(m-1)(p_3 - p_1^2) + mn(n-1)(p_2 - p_1^2)$ where $p_1 = P(X < Y)$, $p_2 = P(X < Y \text{ and } X < Y')$, and $p_3 = P(X < Y \text{ and } X' < Y)$.

$$p_1 = P(X < Y) = \int_{-\infty}^{\infty}\int_{-\infty}^{y} f(x)g(y)\,dx\,dy = p_1 = P(X < Y) = \int_{-\infty}^{\infty} g(y)\int_{-\infty}^{y} f(x)\,dx\,dy =$$

$$\int_{-\infty}^{\infty} g(y)F(y)\,dy = \int_{-\infty}^{\infty} F(y)dG(y) = \int_0^1 udu = \frac{u^2}{2}\bigg|_0^1 = \frac{1}{2}.$$

Under $H_0 : F = G, E(W_{XY}) = \frac{mn}{2}$.

$$p_2 = \int_{-infty}^{\infty}\int_{-\infty}^{\infty}\int_{-infty}^{\infty} f(x)g(y)g(y')\,dx\,dy\,dy',$$

or

$$\int_{-\infty}^{\infty}\int_{x}^{\infty}\int_{x}^{\infty} g(y)g(y')f(x)\,dy\,dy'\,dx = \int_{-\infty}^{\infty} f(x)\int_{x}^{\infty} g(y')\int_{x}^{\infty} g(y)\,dy\,dy'\,dx =$$

$$\int_{-\infty}^{\infty} f(x)[1-G(x)][1-G(x)]\,dx = \int_{-\infty}^{\infty}[1-G(x)]^2\,df = \int_{-\infty}^{\infty}[1-f(x)]^2.$$

Let $u = F(x)$. Then,

$$\int_0^1 (1-u)^2 du = \int_0^1 1 - 2u + u^2 du = \int_0^1 1du - 2\int_0^1 2udu + \int_0^1 u^2 du = 1 - 1 + \frac{1}{3} = p_2$$

under $H_0 : F = G$. To check the variance,

$$Var(W_{XY}) = \frac{mn}{2} + mn(m-1)\left(\frac{1}{3} - \frac{1}{4}\right) + mn(n-1)\left(\frac{1}{3} - \frac{1}{4}\right) = \frac{mn(N+1)}{12}.$$

$$W_{XY} = \sum_{i=1}^{m}\sum_{j=1}^{n}\Phi(x_i, y_j).$$

Let u_{ij} be $\Phi(x_i, y_j)$. Find $E(u_{ij})$.

u	0	1
$P(U = u)$	$1 - p_1$	p_1

$P(U = 1) = P(X < Y)$. $E(u_{ij}) = 0(1-p_1) + 1(p_1) = p_1$. So, $E(W_{XY}) = \sum_{i=1}^{m}\sum_{j=1}^{n} E(u_{ij}) = \sum_{i=1}^{m}\sum_{j=1}^{n} p_1 = mnp_1$.

9.5.5 Calculating Power

$H_0 : \Delta = 0$. $H_1 : \Delta > 0$. $\Delta = E(y) - E(x)$. The power of a test is $P_\Delta(W_{XY} \geq c|H_0)$, which is the probability of rejecting H_0 given the alternative is true. Reject H_0 if $W_{XY} \geq c$.

$$P(W_{XY} \geq c|\Delta) = P\left(\frac{W_{XY} - mnp_1}{\sqrt{Var(W_{XY})}} \geq \frac{c - mnp_1}{\sqrt{Var(W_{XY})}}\right).$$

The power depends on p_1, p_2, p_3. We need an approximate $E_\Delta(W_{XY})$ and $Var_\Delta(W_{XY})$. Consider the shift model. x and $y - \Delta$ are iid with cdf $F(t) = P(x \leq t)$. Thus, $p_1 = P(X < Y) = P(X - Y < 0$. $P(X - (Y - \Delta) < \Delta) = P(X - Y' < \Delta)$ where X, Y' are iid F. Let $F^*(t) = P(X - Y' \leq t)$ be the cdf of $X - Y'$ where X, Y' are iid $F(t)$. Let $f^*(t) = \frac{\partial F^*(t)}{\partial t}$ be the pdf of $X - Y'$.

1. Then, the pdf $f^*(t)$ is symmetric about zero. Recall any random variable which has a distribution symmetric about zero iff $W \overbrace{=}^{\text{ST}} -W$. Check: let $W = X - Y'$. $-W = Y' - X$. Clearly, $W \overbrace{=}^{\text{ST}} -W$ since labeling does not matter.

2. $\lim_{\Delta \to 0} \frac{F^*(\Delta) - F^*(0)}{\Delta}$ is the derivative at Φ which is $f^*(0)$.

3. $F^*(0) = \frac{1}{2}$ because of symmetry. Thus, for small Δ

$$\frac{F^*(\Delta) - F^*(0)}{\Delta} = f^*(0).$$

$$F^*(\Delta) = \Delta f^*(0) + F^*(0) = \Delta f^*(0) \left(\frac{1}{2}\right).$$

$$p_1 = P(X - Y' < \Delta) = F^*(\Delta) = \Delta f^*(0) + \frac{1}{2},$$

if Δ is small. Then,

$$\sqrt{Var(W_{XY})} \approx \sqrt{Var_{H_0}(W_{XY})} = \sqrt{\frac{mn(N+1)}{12}}.$$

Pages 72 and 73 of the text book uses the above approximation to give approximate formulas for the power function. See equation 2.29 and 2.31 in the text book. DO NOT USE THOSE EQUATIONS!

Example: Let $m, n = 10$. Determine the approximate power of the Wilcoxon test of $H_0 : \Delta = 0$. $H_1 : \Delta > 0$. Determine the approximate power at the specific alternative $\Delta = 0.5$ at $\alpha = 0.05$. Assume the shift model where F is the cdf of a Normal distribution where $N(\xi, \sigma^2)$, $\sigma^2 = 32$.

Reject H_0 if $W_{XY} \geq c$.

$$E_{H_0}(W_{XY}) = \frac{mn}{2} = \frac{10(10)}{2} = 50.$$

$$\sqrt{Var_{H_0}(W_{XY})} = \sqrt{\frac{mn(N+1)}{12}} = \sqrt{\frac{10(10)(21)}{12}} = 13.27.$$

Find the critical value $c:$

$$0.05 = P(W_{XY} \geq c) = P(W_{XY} - 0.5 \geq c - 0.5) = P\left(\frac{W_{XY} - 0.5 - 50}{13.27} \geq \frac{c - 0.5 - 50}{13.27}\right) =$$

$$P\left(Z \geq \frac{c - 0.5 - 50}{13.27}\right).$$

Then, $\frac{c-50.5}{13.27} = 1.645$. $c = 72.26$. So, reject H_0 if $W_{XY} \geq 73$. Now, find $P_\Delta(W_{XY} \geq 72.26 | \Delta = 5)$. We need the variance and expectation. The variance is approximated using $Var_{H_0} = 13.27$. However, the expectation does need to be calculated. $E_\Delta(W_{XY}) = mnp_1, p_1 \approx \Delta f^*(0) + \frac{1}{2}$. X, Y' have a Normal distribution, $N(\xi, 32)$. $X - Y' \sim N(0, 262)$. $E(X - Y') = E(X) - E(Y') = 0$. $Var(X - Y') = Var(X) - Var(Y\prime) = 2\sigma^2$.

$$f(t) = \frac{1}{\sigma\sqrt{2\pi}} \exp^{-\frac{1}{2}\frac{(0-0)^2}{2\sigma^2}}$$

Specifically, at $t = 0$ $\frac{1}{\sqrt{2\sigma^2}\sqrt{2\pi}} \approx 0.05$. Now, $p_1 = 5(0.05) + \frac{1}{2} = 0.75$. $E_\Delta(W_{XY}) = mnp_1 = 10(10)(0.75) = 75$. Then, $P\left(\frac{W_{XY}-75}{13.27} \geq \frac{72.26-75}{13.27}\right) = P(Z \geq -0.21) = 0.583$. A small sample size resulted in a small problem solution. Increase m, n.

9.5.6 Confidence Limits for Δ and θ

Recall that $V(\theta) = W_{XY-\theta}$ is a pivotal function. Suppose we want a $(1-\alpha)\%$ confidence interval. Find i, j so that $P_\theta(D_i < \theta < D_j) = 1 - \alpha$. (D_i, D_j) is the confidence interval. i, j must be chosen so that $P_\theta(\theta < D_i) = \frac{\alpha}{2}$ and $P_\theta(\theta > D_j) = \frac{\alpha}{2}$. Remember $V(\theta) = \#$ of differences$(D_i) \leq \theta$. $\theta < D_i \Leftrightarrow \bar{V}(\theta) \leq i-1$. Given $V(\theta)+\bar{V}(\theta) = mn$, then $\theta < D_i \Leftrightarrow mn - V(\theta) = i-1 \Leftrightarrow V(\theta) \geq mn-(i-1) \Leftrightarrow W_{XY-\theta} \geq mn-(i-1)$. $\frac{\alpha}{2} = P_\theta(\theta < D_i) = P_\theta(W_{XY-\theta} \geq mn-i+1) = P_{H_0}(W_{XY} \geq mn-(i-1)) = P_0(W_{XY} \leq i-1) = \frac{\alpha}{2}$. under $\overbrace{Y-\theta}^{\text{ST}}$. We will show that $j = mn-(i-1)$. $D_j < \theta \Leftrightarrow \bar{V}(\theta) \geq j \Leftrightarrow mn - V(\theta) \geq j \Leftrightarrow V(\theta) \leq mn-j \Leftrightarrow W_{XY-\theta} \leq mn-j$. $\frac{\alpha}{2} = P_\theta(D_j < \theta) = P_0(W_{XY} \leq mn-j)$. Therefore, $i-1 = mn-j$. Solving for j, $j = mn-(i-1)$.

Example: A small sample case. $n = 10, m = 7$. Give a 90% confidence interval for θ. Find $i < j$ so that $P_\theta(D_i < \theta < D_j)$. Find the largest i so that $P_\theta(\theta < D_i) = 0.05$. $P_0(W_{XY} \leq i-1)$. From Table B in the text book, $P_0(W_{XY} \leq 17) = 0.439$. Thus, $i-1 = 17 \Rightarrow i = 18$. Then, $j = mn-(i-1) \Rightarrow j = 10(7)-17 = 53$. The confidence interval is (D_{18}, D_{53}). The actual confidence limit is $0.9122 = 1-2(0.0439)$.

Example: A large sample case. $n = m = 20$. Give a 90% confidence interval for the shift parameter θ. Find $i < i$ so that $P_\theta(D_i < \theta < D_j) = 0.90$. Then, $0.05 = P_\theta(\theta < D_i) = P_0(W_{XY} \leq i-1)$. Using the Normal approximation,

$$E_{H_0}(W_{XY}) = \frac{mn}{2} = \frac{20(20)}{2} = 200.$$

$$\sqrt{Var(W_{XY})} = \sqrt{\frac{mn(N+1)}{12}} = \sqrt{\frac{20(20)(41)}{12}} = 37.0$$

$$\Rightarrow P_0(W_{XY} \leq i-1) = P_0(W_{XY} \leq i-1+0.5) = P_)(W_{XY} \leq i-0.5) =$$

$$P_0\left(\frac{W_{XY}-200}{37} \leq \frac{i-0.5-200}{37}\right) = P_0\left(Z \leq \frac{i-200.5}{37}\right).$$

Then, $\frac{i-200.5}{37} = -1.645 \Rightarrow i = 139.64 \approx 139 \Rightarrow j = mn-(i-1) = 20(20)-138 = 262$. The 90% confidence interval is (D_{139}, D_{262}).

9.6 Homework and Answers

Chapter 2.

13(i): $m = n$. $x_1, x_2, ..., x_m$ are iid $N(\xi, \sigma^2)$, $\sigma^2 = 4$. $Y_1 - \Delta$, $Y_2 - \Delta$, ... $Y_n - \Delta$ are iid $N(\xi, \sigma^2)$. $H_0 : \Delta = 0$. $H_1 : \Delta < 0$. $\alpha = 0.01$. Find n so the power is 0.95 when $\Delta = -2$. Ignore the continuity correction.

Solution: Reject H_0 if $W_{XY} \leq c$. If $m = n$ then $E_{H_0}(W_{XY}) = \frac{mn}{2} = \frac{n^2}{2}$. $Var_{H_0}(W_{XY}) = \frac{mn(N+1)}{12} = \frac{n^2(2n+1)}{12}$. We want

$$P_{H_0}(W_{XY} \leq c) = P\left(Z \leq \frac{c-\frac{n^2}{2}}{n\sqrt{\frac{2n+1}{12}}}\right) = 0.01. \Rightarrow c = \frac{n^2}{2} - 2.33\sqrt{\frac{2n+1}{12}}.$$

The power at $\Delta = -2$ is given by

$$P\left(W_{XY} \leq \frac{n^2}{2} - 2.33n\sqrt{\frac{2n+1}{12}}\right).$$

$E_\Delta(W_{XY}) = mnp_1$, $p_1 = 0.5 + \Delta f^*(0)$, $f^*(0) = \frac{1}{2\sqrt{\pi}\sigma} = \frac{1}{4\sqrt{\pi}}$. Then, $p_1 = 0.5 + (-2)\frac{1}{4\sqrt{\pi}} = 0.22$. Thus, $E_\Delta(W_{XY}) = n^2 p_1 = 0.22n^2$ and $Var_\Delta(W_{XY}) = Var_{H_0}(W_{XY})$. Then, the power at $\Delta = -2$ is

$$P\left(Z \leq \frac{\frac{n^2}{2} - 2.33n\sqrt{\frac{2n+1}{12}} - 0.22n^2}{n\sqrt{\frac{2n+1}{12}}}\right) = P\left(Z < \frac{0.28n^2}{n\sqrt{\frac{2n+1}{12}}} - 2.33\right) =$$

$$P\left(Z < \frac{0.28\sqrt{12}n}{\sqrt{2n+1}} - 2.33\right) = 0.95 \Rightarrow \frac{0.28\sqrt{12}n}{\sqrt{2n+1}} - 2.33 = 1.645.$$

After some algebraic manipulations, solve the quadratic equation $0.9408n^2 - 31.6n - 15.8 = 0$ to get $n = 34.08$. Rounding up, use $n = 35$.

23(ii): $m = 20$, $n = 30$. Use the normal approximation to find a 90% confidence interval for Δ. Solution: $E_{H_0}(W_{XY}) = \frac{mn}{2} = 300$. $\sqrt{Var_{H_0}(W_{XY})} = \sqrt{\frac{20(30)(51)}{12}} = 50.5$. $0.05 = P_\Delta(\Delta < D_{(i)}) = P_0(W_{XY} \leq i-1) = P_0(W_{XY} \leq i - 0.5) = \Phi\left(\frac{i-0.5-300}{50.5}\right)$. $\Rightarrow \frac{i-300.5}{50.5} = -1.645$. Solving for i yields, $i = 217.43$. Use $i = 217$. $j = mn - (i-1) = 384$. A 90% confidence interval is $(D_{(217)}, D_{(384)})$.

33: Given that $x_1 \overbrace{>}^{st} x_2$ and $x_2 \overbrace{>}^{st} x_3$, prove $x_1 \overbrace{>}^{st} x_3$. Proof: $x_1 \overbrace{>}^{st} x_2 \Rightarrow P(x_1 > t) \geq P(x_2 > t)$. $x_2 \overbrace{>}^{st} x_3 \Rightarrow P(x_2 > t) \geq P(x_3 > t)$. Both equations imply $P(x_3 > t) \geq P(x_1 > t) \forall t$. Strict inequality holds for some t because strict inequality holds for some t in the equations.

9.7 Mid-term Exam and Answers

1. Consider two treatments and let the response of a subject to treatment A (treatment B) be denoted by $Y(X)$. Assume that X and Y follow the shift model with shift parameter $\Delta = E(Y - X)$. Data on $N = 10$ subjects are shown in the table below.

Trt	Response					
A(Y)	3.89	5.33	5.62	5.70	5.79	Trt
B(X)	1.56	1.89	3.15	3.59	3.96	Control

(a) Determine the value of the Mann-Whitney statistic $W_{XY} = W_s - n(n+1)/2$. The ranks are in parentheses: 1.56(1), 1.89(2), 3.15(3), 3.59(4), 3.89(5), 3.96(6), 5.33(7), 5.62(8), 5.70(9), 5.79(10). W_s = sum of the ranks of the Y's $= 5 + 7 + 8 + 9 + 10 = 39$. $W_{XY} = 39 - \frac{5(6)}{2} = 24$, since $m = n = 5$.

(b) Use Table B to determine the significance probability for testing $H_0 : \Delta = 0$ versus the one-sided alternative $H_1 : \Delta > 0$. Note that $\Delta > 0$ implies that Y is stochastically larger than X. $\hat{\alpha} = P_{H_0}(W_{XY} \geq 24)$. $E_{H_0}(W_{XY}) = \frac{mn}{2} = 12.5$. $P_{H_0}(W_{XY} \leq 1) = 0.0079$.

(c) Use Table B to give an $\alpha = 0.05$ level test of $H_0 : \Delta = 0$ versus the two-sided alternative $\Delta \neq 0$. Express your answer in the form "Reject H_0 if $W_{XY} \leq c_1$, or if $W_{XY} \geq c_2$." That is determine c_1 and c_2. $P_{H_0}(W_{XY} \leq 2) = 0.0159$. Choose $c_1 = 2$ and $c_2 = 12.5 + 10.5 = 23$.

(d) Use the above data to determine the value of the Smirnov statistic $D_{mn} = \max|F_m(t) - G_n(t)|$.

	1.56	1.89	3.15	3.59	3.89	3.96	5.33	5.62	5.70	5.79
mF_m	1	2	3	4	4	5	5	5	5	5
nG_n	0	0	0	0	1	1	2	3	4	5

$D_{mn} = |\frac{4}{5} - \frac{0}{5}| = \frac{4}{5}$.

2. The following data on $N = 100$ subjects was obtained to determine whether a particular treatment tends to decrease the severity of a certain condition.

	Absent	Mild	Severe
Trt	28	12	10
Control	12	15	23
Ties	40	27	33

Determine the value of the Wilcoxon midrank statistic W_s^* = sum of the treatment midranks.

Midrank of Absent: $\frac{d_1+1}{2} = \frac{41}{2} = 20.5$. Midrank of Mild: $d_1 + \frac{d_2+1}{2} = 40 + \frac{28}{2} = 54$. Midrank of Severe: $d_1+d_2+\frac{d_3+1}{2} = 40+27+\frac{34}{2} = 84$. W_s^* = sum of the treatment midranks $= 28(20.5)+12(54)+10(84) = 2062$.

3. In problem #1, assume that the sample sizes are $m = n = 40$. Let $D_{(1)} < \cdots < D_{(mn)}$ denote the ordered differences $Y_j - X_i$. Use the normal approximation and continuity correction to determine $i < j$ so that $D_{(i)}$ and $D_{(j)}$ are lower and upper 95% confidence limits for the shift parameter.

$$E_{H_0}(W_{XY}) = \frac{mn}{2} = \frac{40(40)}{2} = 800.$$

$$\sqrt{Var_{H_0}(W_{XY})} = \sqrt{\frac{mn(N+1)}{12}} = \sqrt{\frac{40(40)(81)}{12}} = 103.92.$$

$$P_\theta(\theta < D_{(i)}) = P_0(W_{XY} \le i-1) = P_0(W_{XY} \le i-1+0.5) = P_0(W_{XY} \le i-0.5) =$$

$$P\left(z \le \frac{i-0.5-800}{103.92}\right) = 0.025 \Rightarrow \frac{i-800.5}{103.92} = -1.96 \Rightarrow i = 596.8.$$

Take $i = 596$. Then, $j = mn - (i-1) = 40(40) - 595 = 1005$.

4. In problem #1, assume that the sample sizes are $m = n = 40$. Consider the problem of testing $H_0 : \Delta = 0$ versus the one-sided alternative $H_1 : \Delta > 0$.

   (a) Use the normal approximation and continuity correction to give an $\alpha = 0.05$ level test. Express your answer in the form "Reject H_0 if $W_{XY} \ge c$."

   $$0.05 = P_{H_0}(W_{XY} \ge c - 0.5) = P\left(Z \ge \frac{c-0.5-800}{103.92}\right) \Rightarrow \frac{c-800.5}{103.92} = 1.645 \Rightarrow c = 971.45.$$

   (b) Assume the X's and Y's have independent normal distributions with common variance $\sigma^2 = 16$. Determine the approximate power of the test in part (a) against the particular alternative $\Delta = 2$. $f^*(0) = \frac{1}{\sqrt{2\pi}\sqrt{2}\sigma} = \frac{1}{2\sqrt{\pi}4} = 0.0705$. $p_1 = 0.5 + 2f^*(0) = 0.5 + 2(0.0705) = 0.6411$. $E(W_{XY}) = mnp_1 = 40(40)(0.6411) = 1025.73$. $\sqrt{Var(W_{XY})} = \sqrt{Var_0(W_{XY})} = 103.92$. The power at $\Delta = 2$ is $P(W_{XY} \ge 971.45) = P\left(Z \ge \frac{971.45-1025.73}{103.92}\right) = P(Z \ge -0.52) = 0.6985$.

   (c) What is meant by the statement that the test in part (a) is unbiased? An unbiased test is one for which $\prod_F(\Delta) \ge \alpha$, for each $\Delta > 0$.

5. The quantity $p_1 = P(X < Y)$ can be written in the form $p_1 = \int_{-\infty}^{\infty} F(t)dG(t)$ where F is the cdf of X and G is the cdf of Y. Assume that F and G are related by $F(t) = [G(t)]^\theta, \forall -\infty < t < \infty$ where θ is a positive constant. Simplify p_1 for this case and write your answer as a simple function of only θ. Hint: The same method used in class for the case $\theta = 1$ will work here. $p_1 = \int_{-\infty}^{\infty} F(t)dG(t) = \int_{-\infty}^{\infty}[G(t)]^\theta dG(t)$. Let $u = G(t)$. Then, $du = dG$ and $p_1 = \int_0^1 u^\theta du = \left.\frac{u^{\theta+1}}{\theta+1}\right|_0^1 = \frac{1}{\theta+1}$.

9.8 Paired Comparisons of Two Treatments

We consider the following paired data tests:

1. The sign test.
2. The Wilcoxon signed rank test.

The general features of a paired data experiment are:

1. N pairs of subjects are available for the experiment.
2. Pairs are formed in one of the following ways:
   (a) Naturally, such as with twins, hands, etc.
   (b) On each subject may serve as his own control such as with before and after treatment measurements on the same subject.
   (c) Or by matching subjects with respect to age, severity of a certain condition, etc.
3. The data takes the form: $(x_1, y_1), (x_2, y_2), ..., (x_N, y_N)$ where Y_i is the treated subject's response and X_i is the control subject's response.
4. Later we introduce the assumption that $(X_i, Y_i), i = 1, 2, ..., N$ are iid pairs so that $Z_i = Y_i - X_i$ are iid differences.

In the randomization model, chance enters only thru random assignment within each pair and independence between pairs.

1. Within each pair, one subject is selected at random(i.e. with probability of one-half) and assigned to the treatment group.
2. The other member is assigned to the control group.
3. If a subject serves as his own control, then it is the order of applying the treatments that is randomly assigned to each subject.
4. The selection of the subject to be assigned to the treatment group is done independently for successive pairs.

The hypotheses tests: H_0 : No treatment difference. H_1 : The treated subjects tend to have a higher response than the controls. Under H_1, the differences $Z_i = Y_i - X_i$ tend to be positive. We may also have left-sided and two-sided alternatives.

9.8.1 The Sign Test

The *sign test* is based on the Binomial distribution. The test statistic is $S_N = \#$ of pairs (x_i, y_i) for which $y_i > x_i = \sum_{i=1}^{N} \phi(x_i, y_i)$ where

$$\phi(x, y) = \begin{cases} 1, & \text{if } y > x \\ 0, & \text{otherwise} \end{cases}$$

9.8.2 Null Distribution of S_N

Under H_0, S_N is the number of successes occurring in N iid trials where $p = P(Y_i - X_i > 0) = 0.5$. That is

$$P_{H_0}(S_N = a) = \binom{N}{a} p^a (1-p)^{N-a}, a = 0, 1, ..., N.$$

Table G in the text book gives the lower tail probabilities for S_N.

9.8.3 Null Mean/Variance and Asymptotic Distribution

$E_{H_0}(S_N) = Np = N(0.5) = \frac{N}{2}$. $Var_{H_0}(S_N) = Np(1-p) = N(0.5)(0.5) = \frac{N}{4}$. The null distribution is symmetric about the mean. In other words, $P_{H_0}\left(S_N \le \frac{N}{2} - c\right) = P_{H_0}\left(S_N \ge \frac{N}{2} + c\right)$. As $n \to \infty$, the standardized form of S_N, namely $\frac{S_N - \frac{N}{2}}{\sqrt{\frac{N}{4}}}$ converges to the standard normal distribution. The continuity correction should be used since the distribution of S_N has equally spaced values $0, 1, 2, ..., N$.

9.8.4 Notation

$N_+ = \#$ of pairs (x_i, y_i) with $y_i - x_i > 0$. $N_0 = \#$ of pairs with $y_i - x_i = 0$. $N_- = \#$ of pairs (x_i, y_i) with $y_i - x_i < 0$. Clearly, $N_+ + N_0 + N_- = N$. N_+, N_0, N_- are random variables.

9.8.5 Conditional Distribution of S_N

In the presence of ties, our test of H_0 is based on N_+. That is, we decide between H_0 and H_1 by examining only those pairs which clearly favor H_1. Let $p_+ = P(Y_i - X_i > 0)$, $p_0 = P(Y_i - X_i = 0)$, and $p_- = P(Y_i - X_i < 0)$. Under H_0, $p_+ = p_-$. The conditional distribution of N_+ given N_0 has a binomial distribution with # of trials $= N - n_0$ parameter $p = P(Y_i - X_i > 0) = 0.5$. We omit the proof.

Example: Page 122 of the text book. $N = 15$ subjects are randomly assigned the order of receiving treatment A(a new drug) or treatment B(a standard drug) for headache relief. The order of receiving the treatment is randomized for each subject on 2 different headache occasions. Suppose $S_N = 10$ subjects report that drug A gives greatest relief. H_0 : no difference in relief, H_1 : drug A gives greater relief than drug B. Reject H_0 if $S_N \ge c$. Using Table G, $\hat{\alpha} = P_{H_0}(S_N \ge 10) = P_{H_0}(S_N \le 5) = 0.1509$ because $|10 - 7.5| = 2.5$ and $|7.5 - 2.5| = 5$. $E_{H_0}(S_N) = \frac{N}{2} = \frac{15}{2} = 7.5$. The significance probability using the Normal approximation is $\hat{\alpha} = P_{H_0}(S_N > 9.5) = P_{H_0}\left(Z \ge \frac{9.5 - 7.5}{1.97}\right) = P(Z \ge 1.03) = 0.151$.

9.9 The Wilcoxon Signed Rank Test

Consider the same situation discussed earlier for the sign test. Pair data: $(x_1, y_1), (x_2, y_2), ..., (x_N, y_N)$ within paired differences: $z_i = y_i - x_i$. H_0 : No treatment response is different. H_1 : The treated subjects tend to have higher responses. We first consider the case of no ties and no zeros. That is, the differences $z_i = y_i - x_i$:

1. Have distinct absolute values $|z_1|, |z_2|, ..., |z_N|$.
2. None of the z_i are equal to zero.

Notation: $N_+ = n =$ # of positive z_i. $N_- = m =$ # of negative z_i. Summary of calculations:

Treatment	y_1	y_2	$\cdots$	y_N
Control	x_1	x_2	$\cdots$	x_N
Differences	z_1	z_2	$\cdots$	z_N
Ordered $\|z_i\|$	$\|z_{(1)}\|$	$\|z_{(2)}\|$	$\cdots$	$\|z_{(N)}\|$
Ranks	1	2	$\cdots$	N

Notation: $S_1, S_2, ..., S_n$ are the ranks of the n positive differences. $R_1, R_2, ..., R_m$ are the ranks of the m negative differences. $N = n + m$. Notes:

1. $\pm 1, \pm 2, ..., \pm N$ are called *signed ranks.*
2. There are 2^N possible ways of attaching signs to the ranks $1, 2, ..., N$.
3. $(S_1, S_2, ..., S_n)$, where there are n observed values of N^+, is that subset of the signed ranks that have positive signs.

4. A special case of $(S_1, S_2, ..., S_n)$ occurs when $n = 0$ ie, when all differences are negative. In this case $(S_1, S_2, ..., S_n)$ is a vector with no elements.
5. $(S_1, S_2, ..., S_{N_+}, N_+)$ varies over subsets of the ranks $\{1, 2, ..., N\}$ where N_+ is the size of the subset selected.
6. N_+ has a binomial distribution with parameters $(N, p), p = 0.5$.

The null distribution of $(S_1, S_2, ..., S_{N_+}, N_+)$: Each combination of signs attached to the ranks corresponds to one value $N_+ = n$ and a set of values $(s_1, s_2, ..., s_n)$ of the ranks of the positive differences. Thus, $P_{H_0}(N_+ = n, S_1 = s_1, S_2 = s_2, ..., S_n = s_n) = \frac{1}{2^N}$. The Wilcoxon Signed Rank Statistic: $N_s = s_1+s_2+\cdots+s_N$ which is the sum of the positive differences. $V_r = r_1+r_2+\cdots+r_m$ which is the sum of the negative differences. Obviously, $V_s + V_r = 1 + 2 + \cdots + N = \frac{N(N+1)}{2}$.

Example: Determine the null distribution of $(N_+, S_1, ..., S_{N_+})$ and V_s when $N = 3$.

Signed Ranks	$(N_+, S_1, ..., S_{N_+})$	V_s	$P_{H_0}(V_s = v)$
1,2,3	3,1,2,3	6	$\frac{1}{8}$
–1,2,3	2,2,3	5	$\frac{1}{8}$
1,–2,3	2,1,3	4	$\frac{1}{8}$
1,2,–3	2,1,2	3	$\frac{1}{8}$
–1,–2,3	1,3	3	$\frac{1}{8}$
–1,2,–3	1,2	2	$\frac{1}{8}$
1,–2,–3	1,1	1	$\frac{1}{8}$
–1,–2,–3	0	0	$\frac{1}{8}$

v	0	1	2	3	4	5	6
P_{H_0}	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{2}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$

This example suggests that in general, the null distribution is symmetric. Properties of the Signed Rank statistic:

1. V_s and V_r have the same null distribution. Clearly true because we can replace each positive rank by a negative rank and leave the distribution unchanged.
2. $E_{H_0}(V_s) = \frac{N(N+1)}{4}$. proof: $V_s + V_r = \frac{N(N+1)}{2} \to E_{H_0}(V_s) + E_{H_0}(V_r) = \frac{N(N+1)}{2}$. By property (1), $E_{H_0}(V_s) = E_{H_0}(V_r)$. Thus, $2E_{H_0}(V_s) = \frac{N(N+1)}{2} \Rightarrow E_{H_0}(V_s) = \frac{N(N+1)}{4}$.
3. The null distribution of V_s is symmetric about $E_{H_0}(V_s) = \frac{N(N+1)}{4}$. proof: The largest possible value of V_s occurs when all of the $z_i = y_i - x_i$ are positive. In this case $V_s = 1 + 2 + \cdots + N = \frac{N(N+1)}{2}$. The smallest possible value of V_s occurs when none of the z_i are positive. In this case, $V_s = 0$. Thus, V_s takes the values $0, 1, 2, ..., k$ where $k = \frac{N(N+1)}{2}$. Note that $E_{H_0}(V_s) = \frac{N(N+1)}{4}$ is the center of this set. But, $V_s + V_r = k \Rightarrow P_{H_0}(V_s = a) = P_{H_0}(k - V_r = a) = P_{H_0}(V_r = k - a) = P_{H_0}(V_s = k - a)$ by property (1). This proves symmetry.
4. Table H in the text book gives lower tail probabilities $P_{H_0}(V_s \leq a)$, for $N \leq 20$. Symmetry can be used to get upper tail probabilities.
5. Under H_0, $V_s = \sum_{i=1}^{N} a_i V_i$ where $a_i = i, i = 1, 2, ..., N, V_1, V_2, ..., V_N$ are iid Bernoulli random variables.

$$V_i = \begin{cases} 1, & \text{if } Y_i - X_i > 0 \\ 0, & \text{otherwise} \end{cases}$$

$P(V_i = 1) = P(V_i = 0) = \frac{1}{2}$. That is, under H_0 V_s is distributed like the total of a sample of size N drawn from the population $\{1, 2, ..., N\}$ by binomial sampling. Each $a_i = i$ in the population is included in the sample with probability of $\frac{1}{2}$.

6. It is easy to use property (5) to determine the null mean and variance of V_s. $E_{H_0}(V_s) = \frac{N(N+1)}{4}$, and $Var_{H_0}(V_s) = \frac{N(N+1)(2N+1)}{24}$. proof: $Var_{H_0}(V_s) = \sum_{i=1}^{N} a_i^2 Var(V_i)$, $Var(V_i) = p(1-p) = \frac{1}{2}\left(1-\frac{1}{2}\right) = \frac{1}{4}$. $\Rightarrow Var_{H_0}(V_s) = \sum_{i=1}^{N} i^2\left(\frac{1}{4}\right)$. By exercise 84, Chapter 1 of the text book, $\sum_{i=1}^{N} i^2 = \frac{N(N+1)(2N+1)}{6}$. Thus, $Var_{H_0}(V_s) = \frac{1}{4}\sum_{i=1}^{N} i^2 = \frac{N(N+1)(2N+1)}{24}$.

7. As $N \to \infty$, $\frac{V_s - E_{H_0}(V_s)}{\sqrt{Var_{H_0}(V_s)}}$ converges to a standard Normal random variable(theorem 5, text book appendix).

Example: $N = 10$ pairs.

Treatment										
$A(y)$	659	984	397	574	447	479	676	761	647	577
$B(x)$	452	587	460	787	351	277	234	516	577	513
$z = y - x$	207	397	–63	–213	96	202	442	245	70	64
$\lvert z_i \rvert$	207	397	63	213	96	202	442	245	70	64
Ranks	6	9	1	7	4	5	10	8	3	2
Signed Rank	6	9	–1	–7	4	5	10	8	3	2

$V_s = 6+9+4+5+10+8+3+2 = 47$. H_0 : no treatment effect. $H_1 : z_i = y_i - x_i$ tend to be positive. Reject H_0 if $V_s \geq c$. The significance probability using Table H is $E_{H_0}(V_s) = \frac{N(N+1)}{4} = \frac{10(11)}{4} = 27.5$. $\hat{\alpha} = P_{H_0}(V_s \geq 47) = P_{H_0}(V_s \leq 27.5 - 19.5) = P(V_s \leq 8) = 0.0244$. The significance probability using the Normal approximation and continuity correction is

$$E_{H_0}(V_s) = \frac{N(N+1)}{4} = \frac{10(11)}{4} = 27.5.$$

$$\sqrt{Var_{H_0}(V_s)} = \sqrt{\frac{N(N+1)(2N+1)}{24}} = \sqrt{\frac{10(11)(21)}{24}} = 9.81.$$

$$\hat{\alpha} = P_{H_0}(V_s \geq 47) = P_{H_0}(V_s \geq 46.5) = P\left(Z \geq \frac{46.5 - 27.5}{9.81}\right) = P(Z \geq 1.94) = 0.0262.$$

Comparison with the sign test: In the previous example, $S_n = \#$ of positive differences $= 8$. $\hat{\alpha} = P_{H_0}(S_n \geq 8) = 1 - P_{H_0}(S_n \leq 7) = 1 - 0.945 = 0.055$. Thus, the result is not as significant with the sign test. The sign test ignores certain information and should not be used if the different $z_i's$ are observable. An alternative representation of the signed rank test statistic(used in chapter 4 of the text book) is to let $z_i = y_i - x_i, i = 1, 2, ..., N$. Consider all averages $\frac{z_i + z_j}{2}, i \leq j$. The total number of such pairwise averages is $\begin{pmatrix} N \\ 2 \end{pmatrix} + N$. We will show that $V_s = \#$ of pairs $(z_i, z_j), i \leq j$, for which $\frac{z_i + z_j}{2} > 0$. proof: We start with RHS and show it equals LHS. $RHS = \sum\sum_{i \leq j} I\left(\frac{z_i + z_j}{2} > 0\right)$, where

$$I(A) = \begin{cases} 1, & \text{if event A holds.} \\ 0, & \text{otherwise.} \end{cases}$$

$$RHS = \sum_{j=1}^{N}\sum_{i=1}^{j} I\left(\frac{z_i + z_j}{2} > 0\right).$$

To simplify this last expression, let $z_1, z_2, ..., z_N$ be labeled so that $|z_1| < |z_2| < ... < |z_N|$. Then, $z_j > 0 \Leftrightarrow \frac{z_i + z_j}{2} > 0, \forall i \leq j$. Using (*) we have

$$\sum_{i=1}^{j} I\left(\frac{z_i + z_j}{2} > 0\right) = \begin{cases} 1, & \text{if } z_i > 0. \\ 0, & \text{if } z_i < 0. \end{cases}$$

Thus, $\sum_{i=1}^{j} I\left(\frac{z_i+z_j}{2} > 0\right) = jI(z_j > 0)$. We have $RHS = \sum_{j=1}^{N}\sum_{i=1}^{j} I\left(\frac{z_i+z_j}{2} > 0\right) = \sum_{i=1}^{N} jI(z_j > 0) = V_s$.

9.9.1 Correction for Ties V_s

The correction for ties and zeros is similar to that of the rank sum statistic of Chapter 1 and 2 in the text book and the sign rank statistic.

Example: $N = 7$.

Treatment							
$A(Y)$	0	0	0	2	0	1	0
$B(X)$	–1	–2	1	2	0	–1	0
$z = y - x$	1	2	–1	0	0	2	0
$\lvert z_i \rvert$	1	2	1	0	0	2	0
Midranks	4.5	6.5	4.5	2	2	6.5	2
Signed Midranks	4.5	6.5	–4.5	0	0	6.5	0

Note: the signed midranks are calculated by multiplying the midranks by $+1, -1, 0$ according to whether z_i is $+, -$ or zero. $V_s^* =$ sum of positive midranks $= 4.5 + 6.5 + 6.5 = 17.5$. We cannot use Table H to obtain critical values or a significance probability

9.9.2 Asymptotic Null Distribution of V_s^*

Tables of the null distribution of V_s^* are not practical to construct. So we must rely on the Normal approximation. Notation: e is the number of nonzero distinct values of $|z_1|, |z_2|, ..., |z_N|$. $d_0 =$ the number of $z_i = 0$. $d_i =$ the number of $|z_i|$ that are tied at the $i-th$ largest of the $|z_i|$. $N' = N - d_0$ which is the number of nonzero z_i.

$\lvert z_i \rvert$	# of tied values	midranks
0	d_0	$(d_0+1)/2$
$\lvert z_1 \rvert$	d_1	$d_0 + (d_1+1)/2$
$\lvert z_2 \rvert$	d_2	$d_0 + d_1 + (d_2+1)/2$
.	.	.
.	.	.
.	.	.
$\lvert z_e \rvert$	d_e	$d_0 + d_1 + \cdots + (d_e+1)/2$

Define the constants $a_1, a_2, ..., a_{N'}$ as the midranks corresponding to the nonzero differences. That is $a_1 = a_2 = \cdots = a_{d_1} = d_0 + \frac{d_1+1}{2}$. $a_{d_1+1} = a_{d_1+2} = \cdots = a_{d_1+d_2} = d_0 + d_1 + \frac{d_2+1}{2}$. ... With this definition of $a_1, a_2, ..., a_{N'}$ we have $V_s^* = a_1v_1 + a_2v_2 + \cdots + a_{N'}v_{N'}$ where $v_1, v_2, ..., v_{N'}$ are iid Bernoulli random variables such that $P(V_i = 1) = \frac{1}{2}$ and $P(V_i = 0) = \frac{1}{2}$. Since by * we have V_s^* as a linear function of independent random variables. It is easy to calculate the mean and variance of V_s^*. We omit further details and state the following: $E_{H_0}(V_s^*) = \frac{N(N+1)}{4} - \frac{d_0(d_0+1)}{4}$. $Var_{H_0}(V_s^*) = \frac{N(N+1)(2N+1) - d_0(d_0+1)(2d_0+1)}{24} - \sum_{i=1}^{e} \frac{d_i(d_i^2-1)}{48}$.

Example: This is Example 4 on page 131 of the text book. There are $N = 12$ matched pairs. $z_i = treatment - control$ which is the gain in IQ over a 6 week period.

z_i	6	–8	9	5	–7	5	–3	3	–12	3	0	–1
$\|z_i\|$	6	8	9	5	7	5	3	3	12	3	0	1
midranks	8	10	11	6.5	9	6.5	4	4	12	4	1	2

V_s^* = sum of the midranks of the + differences = 40. H_0 : no treatment effect, H_1 : treatment response tends to be larger than the control. Reject H_0 if $V_s^* \geq c$. $e = 8$, $d_0 = 1$, $d_2 = 3$, $d_3 = 2$ and all other $d_i = 1$.

$$E_{H_0}(V_s^*) = \frac{N(N+1)}{4} - \frac{d_0(d_0+1)}{4} = \frac{12(13)}{4} - \frac{1(2)}{4} = 38.5.$$

$$Var_{H_0}(V_s^*) = \frac{N(N+1)(2N+1) - d_0(d_0+1)(2d_0+1)}{24} - \sum_{i=1}^{e} \frac{d_i(d_i^2-1)}{48} =$$

$$\frac{12(13)(25) - 1(2)(3)}{24} - \frac{30}{48} = 161.625.$$

Then,

$$\hat{\alpha} = P_{H_0}(V_s^* \geq 40) = P\left(Z \geq \frac{40-38.5}{12.71}\right) = P(z \geq 0.118) = 0.453.$$

9.10 Population Models/The One Sample Problem

Since the objective of an experiment is to make inferences about a population, the pairs of subjects must be randomly selected from the population. Population Model:

1. N pairs of subjects are randomly selected from a population of pairs.
2. One subject in each pair is randomly assigned to the treatment group, and the other subject to the control group; ie, the assignment is made independently between pairs and a particular member of each pair has probability 0.5 of begin assigned to the treatment group.

As in Chapter 3 of the text book, Y_i is the response of the treated subject in the i-th pair and X_i is the response of the control subject in the i-th pair. Although we often refer to treatment and control groups, it is clear that one group may receive treatment A and the other group receive treatment B. If the population size is large in comparison to the sample size, then a sample of N pairs of subjects taken *without replacement* can be treated as if dependence between pairs is negligible. Thus, an infinite population model implies the following:

1. $(x_1, y_1), (x_2, y_2), ..., (x_N, y_N)$ are iid pairs with a common bivariate cdf $M(x, y) = P(X \leq x, Y \leq y)$.
2. $z_1, z_2, ..., z_N$ are iid random variables with some cdf $L(x) = P(Z \leq x)$.
3. If $M(x, y)$ is a continuous bivariate distribution with dome joint pdf, then $L(x)$ will also be a continuous distribution with some pdf.

In Chapter 4 of the text book, our discussion will primarily use the fact that $z_1, z_2, ..., z_N$ are iid with some cdf $L(x) = P(Z \leq x)$. $L(x)$ being continuous implies that ties and zeros occur with probability zero. In Chapter 3 of the text book, the null and alternative hypotheses were H_0 : No treatment effect; H_1 : The treated subject's response tends to be higher than the control subject's response.

We now state H_0 in the form: H_0 : $L(x)$ is symmetric about zero. Since the mean of a symmetric distribution must equal the point of symmetry, we have $E_{H_0}(z_i) = 0$. The pdf of a continuous distribution, symmetric about zero, may look like the standard normal curve. Symmetry about zero implies $P(Z > x) = P(Z < -x), \forall -\infty < x < \infty$. In terms of the cdf $L(x) = P(Z \leq x)$, we see that Z has a continuous distribution symmetric about zero if and only if $1 - L(x) = L(-x), \forall -\infty < x < \infty$. Definition: The random variable Z, with cdf $L(x)$, has a distribution symmetric about zero if $L(x) + L(-x) = 1, \forall -\infty < x < \infty$.

The alternative hypothesis that the treated subject's response tends to be higher than the control subject's response suggests that the z_i will tend to take positive values.

Definition: Let Z have cdf $L(x) = P(Z \leq x)$. We say that Z is stochastically positive if $P(Z > x) \geq P(Z < -x), \forall -\infty < x < \infty$ and if strict inequality holds for some x. The pdf of a stochastically positive random variable may look like the following: $\Delta = E(z)$

```
\ |                            |   /  /
\ |                            | /  /
\ |                            |  /
--|-------------|---------------|-------
 -x             0               x
```

This distribution is stochastically positive because for every x, the area under the pdf to the right of x is greater than the area to the left of $-x$. In terms of the cdf $L(x) = P(Z \leq x)$, note that the condition * can be written $1 - L(x) \geq L(-x), \forall - \infty < x < \infty$. Thus, an equivalent definition of a stochastically positive random variable is the following: Let Z have cdf $L(x) = P(Z \leq x)$. We say Z is stochastically positive if $L(x) + L(-x) \leq 1, \forall - \infty < x < \infty$ and if strict inequality holds for some x. By comparing this definition with the one given earlier for a symmetric distribution, we see that if equality holds in this definition for all x, then $L(x)$ is symmetric about zero. We could define Z to be *stochastically negative* if $L(x) + L(-x) \geq 1, \forall - \infty < x < \infty$ and if strict inequality holds for some x. *Distributions symmetric about zero are a boundary between the class of stochastically positive random variables and the class of stochastically negative random variables.*

9.10.1 Shift Model

We say that the differences $Z = Y - X$ follow the shift model with shift parameter $\Delta = E(Z) = E(Y - X)$ if $Z \overbrace{=}^{\text{ST}} U + \Delta$ where u has a distribution symmetric about zero. Notation used in the text book: $\overbrace{E(x) = P(U \leq x)}^{\text{not expectation}}$ is the cdf of a distribution symmetric about zero. $L(x) = P(Z \leq x)$ is the cdf of the $z's$.

Example: If u has a Normal distribution with mean of zero and variance σ^2, then $Z \overbrace{=}^{\text{ST}} u+\Delta$ has a Normal distribution with mean Δ and variance σ^2. This is a particular case of the shift model. An equivalent form of the shift model is, $L(t) = P(Z \leq t) = P(u + \Delta \leq t) = P(u \leq t - \Delta) = E(t - \Delta)$. Thus, the shift model is equivalently described by the requirement that $L(x) = E(X - \Delta), \forall - \infty < x < \infty$ where Δ is a constant. $E(x)$ is the cdf of a distribution symmetric about zero.

Assume that Z follows the shift model. Then,

1. $\Delta = 0 \Rightarrow Z$ has a distribution symmetric about zero.
2. $\Delta > 0 \Rightarrow Z$ is stochastically positive.
3. $\Delta < 0 \Rightarrow Z$ is stochastically negative.

Thus under the shift model, the null and alternative hypotheses can be written in the form: $H_0 : \Delta = 0$, $H_1 : \Delta > 0$. Of course, we may also have a left-sided alternative or a two-sided alternative. Note: under the shift model, u has a *general* symmetric distribution and, in this sense, the shift model is "non-parametric."

9.10.2 Estimating the Shift Parameter

Before considering the shift parameter, let us first consider the following more common situations:

1. The one-sample t-statistic. Recall that if $\bar{X}$ is the mean of a sample of n observations from a population of measurements that have a normal distribution, $N(\theta, \sigma^2)$, then $T(\theta) = \frac{\bar{X}-\theta}{s/\sqrt{n}}$ has a t-distribution with $n - 1$ degrees of freedom. The mean of the distribution of $T(\theta)$ is $E_\theta[T(\theta)] = 0$. One way to estimate θ is to equate $T(\theta)$ to the mean equal to zero of the distribution of $T(\theta)$. Thus, $T(\theta) = 0 \Rightarrow \frac{\bar{X}-\theta}{s/\sqrt{n}} = 0$ $\Rightarrow \hat{\theta} = \bar{X}$.

2. Maximum likelihood estimation. Let $x_1, x_2, ..., x_n$ be iid with some pdf $f(x, \theta)$ that depends on a parameter θ. The likelihood function is

$$L(\theta) = \prod_{i=1}^{n} f(x_i, \theta).$$

The log of the likelihood function is

$$\log L(\theta) = \prod_{i=1}^{n} \log f(x_i, \theta).$$

The derivative of the log likelihood function is

$$u(\theta) = \frac{\partial}{\partial \theta} \log L(\theta) = \sum_{i=1}^{n} \frac{\partial}{\partial \theta} \log f(x_i, \theta).$$

This last expression shows that $u(\theta)$ is a sum of iid random variables. It is well known that $u(\theta)$ has asymptotically ($n \to \infty$) a normal distribution with mean $E[u(\theta)] = 0$. The maximum likelihood estimator $\hat{\theta}$ of θ is obtained by solving the equation $u(\theta) = 0 =$ point of symmetry of the limiting distribution. We will use the Mann-Whitney statistic to estimate the shift parameter in a similar way.

Following the previous examples, let us denote the shift parameter by θ. We will sometimes think of θ as being the true value of the shift parameter. Other times, we interpret θ as just being a variable argument of a function. Let $V(\theta) = W_{x,y-\theta} = \#$ of pairs (x_i, y_j) for which $x_i < y_j - \theta = \#$ of pairs $x_i, y_j)$ for which $y_j - x_i > \theta$. $\bar{V} = \#$ of pairs (x_i, y_j) for which $y_j - x_i \leq \theta$. Now $V(\theta)$ and $\bar{V}(\theta)$ are functions of the variable θ. Note that:

1. $V(\theta) + \bar{V}(\theta) = mn$.
2. $\bar{V}(\theta)$ is a right continuous, non-decreasing step function, similar to a cdf.
3. $V(\theta)$ is a right continuous, non-increasing step function.

Because $\bar{V}(\theta)$ is similar to a cdf, it will be easier for us to work in terms of $\bar{V}(\theta)$. Let $D_{(1)} < D_{(2)} < \cdots < D_{(mn)}$ be the ordered set of mn differences $y_j - x_i$. To get a point estimate of θ, we must equate $W_{x,y-\theta}$ to the mean of its distribution. If θ is the true value of the shift parameter, then $X_1, X_2, ..., X_m$ and $Y_1 - \theta, Y_2 - \theta, ..., Y_n - \theta$ are all iid with common cdf $F(t)$. Thus $E_\theta(W_{x,y-\theta}) =$ mean of the null distribution of the Mann-Whitney statistic $= \frac{mn}{2}$. In order to solve the equation $V(\theta) = W_{x,y-\theta} = \frac{mn}{2}$ for $\hat{\theta}$, we need the following theorem:

Theorem: Page 87 of the text book. I the differences $Y_j - X_i$ are all distinct and have the ordered values $D_{(1)} < D_{(2)} < \cdots < D_{(mn)}$ then

1. $D_{(i)} \leq \theta \Leftrightarrow V(\theta) \leq mn - i$.
2. $D_{(i)} \leq \theta < D_{(i+1)} \Leftrightarrow V(\theta) = mn - i$.

Proof: Part (1): Recall that $V(\theta) + \bar{V}(\theta) = m$. Thus $D_{(i)} \leq \theta \Leftrightarrow \bar{V}(\theta) \geq i \Leftrightarrow mn - V(\theta) \geq i \Leftrightarrow V(\theta) \leq mn - i$. Part (2): $D_{(i)} \leq \theta \leq D_{(i+1)} \Leftrightarrow \bar{V}(\theta) = i \Leftrightarrow mn - V(\theta) = i \Leftrightarrow V(\theta) = mn - i$.

We now want to solve the equation, $V(\theta) = \frac{mn}{2}$. The solution to this equation denoted by $\hat{\theta}$ is called the *Hodges-Lehmann estimator* of the shift parameter. The equation $V(\theta) = \frac{mn}{2}$ only has an approximate solution. There are two cases:

Case 1: mn is an even integer. That is, $mn = 2k$ for some integer k. Solve the equation $V(\theta) = k$ By the previous theorem, part (2), $D_{(k)} \leq \theta < D_{(k+1)} \Leftrightarrow V(\theta) = mn - k \Leftrightarrow V(\theta) = 2k - k = k$. Thus, if $mn = 2k$, then the solution to $V(\theta) = \frac{mn}{2}$ is any number θ in the interval $D(k) \leq \theta < D_{(k+1)}$. We take as our solution $\hat{\theta} = \frac{D_{(k)} + D_{(k+1)}}{2} =$ median of the set $D_{(1)}, ..., D_{(mn)}$.

Case 2: mn is an odd integer. Then $mn = 2k+1$ for some integer k. By the previous theorem, part (2), $D_{(k)} \leq \theta < D_{(k+1)} \Leftrightarrow V(\theta) = mn - k \Leftrightarrow V(\theta) = (2k+1) - k = k+1$ and $D_{(k+1)} \leq \theta < D_{(k+2)} \Leftrightarrow V(\theta) mn - (k+1) \Leftrightarrow V(\theta) = (2k+1) - (k+1) = k$. Thus the equation

$$V(\theta) = \frac{mn}{2} = \frac{2k+1}{2} = k + \frac{1}{2}$$

has no solution. The closest we can get to a solution is to take $\hat{\theta} = D_{(k+1)}$ = median of the set $D_{(1)}, D_{(2)}, ..., D_{(mn)}$ when mn is an odd integer.

9.10.3 Power of the Sign Test

The hypotheses are: $H_0 : \Delta = 0$, $H_1 : \Delta > 0$. The sign statistic is

$$S_n = \#(z_i > 0) = \sum_{i=1}^{N} I(z_i > 0),$$

where

$$I(z_i > 0) = \begin{cases} 1, & \text{if } z_i > 0. \\ 0, & \text{otherwise} \end{cases}$$

S_N has a binomial distribution with parameter $p = P(z_i > 0)$. Under H_0 $p = 0.5$. For a specified α level test, we reject H_0 if $S_N \geq k$ where k is a positive integer obtained from Table G in the text book. The power of the α level test against a particular alternative $\Delta > 0$ is $\prod_F(\Delta) = P_\Delta(S_N \geq k)$ the distribution of S_N depends on Δ only through the parameter p. $\Delta = 0 \Rightarrow p = 0.5 \Rightarrow \prod_F(0) = \alpha$. $\Delta > 0 \Rightarrow p = P(Z > 0) = P(u + \Delta > 0) = P(u > -\Delta) > 0.5$. Recall that $P(S_N \geq k) = \int_0^p f_k(x)\,dx$ where $f_k(x)$ is the pdf of the $k-th$ order statistic in a sample of size N from a uniform distribution on the interval $(0, 1)$. Thus, $P(S_N \geq k)$ is an increasing function of p. Thus, the test if unbiased because $\alpha = \prod_F(0) \leq \prod_F(\Delta), \forall \Delta > 0$.

Example: On page 160 of the text book, the example illustrates calculating the power of the sign test. For a specified $\Delta > 0$, we calculate $p = P_\Delta(Z > 0) = P(u > -\Delta)$, then

$$\prod_F(p) = P\left(\frac{S_N - NP}{\sqrt{Np(1-p)}} \geq \frac{k - Np}{\sqrt{Np(1-p)}}\right)$$

and a continuity correction would be used.

Example: On page 160 of the text book. In this example, the Z_i do not arise from paired data. However, we assume that the Z_i follow the shift mode $Z = u + \Delta$. Then, Z has a distribution symmetric about Δ. That is, $E(Z) = \Delta$. The hypotheses are $H_0 : \Delta = 22$, $H_1 : \Delta < 22$. Reject if $S_N \geq c$.

9.10.4 Approximate Power of the Sign Test

We assume that the differences $z_1, z_2, ..., z_N$ follow the shift model:

- $z_1, z_2, ..., z_N$ are iid.
- $z_i \overbrace{=}^{\text{ST}} u_i + \Delta, i = 1, 2, ..., N$ where the u_i has a continuous distribution symmetric about zero.

In simple terms, the shift model implies the z_i have a distribution symmetric about $\Delta = E(z_i)$. This distribution could be the Normal but includes many other cases. Consider the problem of testing the hypotheses

$\Delta = 0$, $H_1 : \Delta > 0$. The test statistic is V_s which is the number of pairs $(z_i, z_j), i \leq j$ for which $z_i + z_j > 0$. Under H_1, the z_i will tend to have large positive values and consequently V_s will tend to take large values. Reject H_0 if $V_s \geq c$ where $P_{H_0}(V_s \geq c) = \alpha$.

Example: A new treatment is to be tested for its effectiveness in lowering the blood pressure using a sample of $N = 25$ subjects. Let $z_i = before - after$ differences in blood pressure of the subjects. If the treatment is truly effective, then the z_i will tend to be positive. Consider the problem of testing $H_0 : \Delta = 0$ versus $H_1 : \Delta > 0$ where $\Delta = E(z_i)$ is the mean change in blood pressure, using the signed rank test.

1. Use the Normal approximation to a given $\alpha = 0.05$ level test in the form reject H_0 if $V_s \geq c$.

2. Assuming the z_i have a Normal distribution with variance $\sigma^2 = 4$, determine the approximate power of the test in part (1) against the alternative $\Delta = 1.0$.

Solution:

1. $E_{H_0}(V_s) = \frac{N(N+1)}{4} = \frac{25(26)}{4} = 162.5$. $\sqrt{Var_{H_0}(V_s)} = \sqrt{\frac{N(N+1)(2N+1)}{24}} = \sqrt{\frac{25(26)(51)}{24}} = 37.165$.

$$0.05 = P_{H_0}(V_s) \geq c) = P_{H_0}(V_s \geq c - 0.5) = P\left(z \geq \frac{c - 0.5 - 162.5}{37.165}\right) = 0.05.$$

$$\Rightarrow \frac{c - 163}{37.165} = 1.645 \Rightarrow c = 224.14.$$

Reject H_0 if $V_s \geq 225$.

2.

$$E_\Delta(V_s) = \left(\begin{array}{c} N \\ 2 \end{array}\right) p_1' + Np.$$

$\sqrt{Var_\Delta(V_s)} \approx \sqrt{Var_{H_0}(V_s)} = 37.165$. $p = P_\Delta(z_i > 0), z_i \sim N(\Delta, 4)$ where $\Delta = E(z) = 1.0$.

$$p = P\left(\frac{z_i - 1}{2} > \frac{0 - 1}{2}\right) = P(W > -.5) = 0.6915.$$

$$p_1' = P_\Delta(z_i + z_j > 0), z_i + z_j \sim N(2\Delta, 2\sigma^2).$$

$$p_1' = P_\Delta\left(\frac{z_i + z_j - 2}{\sqrt{8}} > \frac{0 - 2}{\sqrt{8}}\right) = P(W > -0.71) = 0.7611.$$

$$\left(\begin{array}{c} N \\ 2 \end{array}\right) = E_\Delta(V_s) = \left(\begin{array}{c} 25 \\ 2 \end{array}\right) = 300.$$

$$E_\Delta(V_s) = (300)(0.7611) + (25)(0.6915) = 245.62.$$

The power is given by

$$P_\Delta(V_s \geq 224.14) = P\left(Z \geq \frac{224.14 - 245.62}{37.165}\right) = P(Z \geq -0.58) = 0.7190.$$

9.10.5 Estimating a Location Parameter

In this section we derive the Hodges-Lehmann estimator of the population median and of the center of symmetry of a continuous symmetric distribution. $\theta = E(z_i) = \Delta$. Get the Hodges-Lehmann estimator of θ. Let $z_1, z_2, ..., z_n$ be iid with a continuous cdf $L(x) = P(z_i = x)$. θ is a unique median. Let $S_N(z-\theta) = \#(z_i - \theta > 0) = \#(z_i > 0)$. If θ is the true value of the population median, then $p = P(z_i > \theta) = 0.5$. So, $S_N(z-\theta)$ is $Binomial(N, 0.5)$.

$$E(S_N(z-\theta)) = Np = \frac{N}{2}.$$

When N is even, there is an infinite number of solutions. When N is odd, there are no solutions.

Theorem: Let $z_1 < z_2 < \cdots < z_n$ be N distinct ordered values of the z_i. For any integer, $1 \leq i \leq N$,

1. $z_{(i)} \leq \theta \Leftrightarrow S_N(z-\theta) \leq N-i$.
2. $z_{(i)} > \theta \Leftrightarrow S_N(z-\theta) \geq N-i+1$.
3. $z_{(i)} \leq \theta < z_{(i+1)} \Leftrightarrow S_N(z-\theta) = N-i$.

The Hodges-Lehmann estimator of the median is the solution to the equation, $S_N(z-\theta) = \frac{N}{2}$.

Case 1: N is an even integer. By the above theorem, $z_{(N/2)} \leq \theta < z_{(N/2+1)}$. Then, $S_N(z-\theta) = N - i = N - \frac{N}{2} = \frac{N}{2}$. Then, $\hat{\theta}$ is the average of the two middle values which is the median of $(z_1, z_2, ..., z_n)$.

Case 2: N is an odd integer. Then $N = 2r+1 \Rightarrow \frac{N}{2} = \frac{2r+1}{2} = r + \frac{1}{2}$. $S_N(z-\theta) = \frac{N}{2} = r + \frac{1}{2}$. The closest we can get is r or $r+1$. By the theorem, if $z_{(r)} \leq \theta < z_{(r+1)} \Rightarrow S_N(z-\theta) = N - r = 2r+1-r = r+1$. If $z_{(r+1)} \leq \theta < z_{(r+2)} \Rightarrow S_N(z-\theta) = N-(r+1) = (2r+1)-(r+1) = r \Rightarrow \hat{\theta} = z_{(r+1)}$.

9.10.6 Estimating the Center of Symmetry θ

We will estimate the center of symmetry of a continuous symmetric distribution. Let $V_s(z-\theta)$ be the number of pairs $(z_i - \theta, z_j - \theta), i \leq j$ for which $\frac{(z_i-\theta)+(z_j-\theta)}{2} > 0 =$ the number of pairs $(z_i, z_j), i \leq j$ for which $\frac{z_i+z_j}{2} > \theta$. Note that the first expression emphasizes that $V_s(z-\theta)$ is also a function of the averages $\frac{z_i+z_j}{2}, i \leq j$. Let $A_{(1)}, A_{(2)}, ..., A_{(N)}$ denote the ordered averages. How many such averages are there?

$$M = \binom{N}{2} + N$$

as noted earlier, when deriving the expected value of V_s. Recall that the null mean of the signed rank statistic is $E_{H_0}(V_s) = \frac{N(N+1)}{4}$. To express this mean in terms of M, note that $M = \binom{N}{2} + N = \frac{N(N-1)}{2} + N = \frac{N(N+1)}{2}$. So, $\frac{M}{2} = \frac{N(N+1)}{4} = E_{H_0}(V_s)$. The Hodges-Lehmann estimator of the shift parameter(based on the signed rank statistic) is the approximate solution to the equation $V_s(z-\theta) = \frac{M}{2}$. The approximate solution to that equation is $\hat{\theta} = median(A_i) = median\left(\frac{z_i+z_j}{2}\right)_{i \leq j}$ and is obtained in exactly the same way as in the case of the sign statistic. As noted on page 180 of the text book, $\hat{\theta}$ is a more efficient estimator than $\tilde{\theta}$.

9.10.7 More on the Signed Rank Statistic

The expected value and the variance of the signed rank statistic will be calculated for the general case. The assumptions are $z_1, z_2, ..., z_N$ are iid with continuous cdf $L(x) = P(Z \leq x)$. $L(x)$ being continuous implies that there are no ties and no zeros. V_s is the Wilcoxon signed rank statistic which is # of pairs $(z_i, z_j), i \leq j$ for which $\frac{z_i+z_j}{2} > 0 =$ # of pairs $z_i, z_j), i \leq j$ for which $z_i + z_j > 0 = \sum\sum_{i\leq j} V_{ij} = V_{ij} = \phi(z_i, z_j)$ where

$$\phi = \begin{cases} 1, & \text{if } u + v > 0. \\ 0, & \text{otherwise.} \end{cases}$$

The expected value and variance are: $E(V_s) = \begin{pmatrix} N \\ 2 \end{pmatrix} p_1' + Np$. $Var(V_S) = N(N-1)(N-2)[p_2' - (p_1')^2]+$ $Np(1-p) + \frac{N(N-1)}{2}\left[2(p-p_1')^2 + 3p_1'(1-p_1')\right]$, where $p = P(Z_i > 0)$, $p_1' = P(Z_i + Z_j > 0), i \neq j$, and $p_2' = P(Z_i + Z_j > 0 \text{ and } Z_i + Z_k > 0), i \neq j \neq k$. Since $z_1, z_2, ..., z_N$ are iid, the parameters p, p_1', p_2' can also be written as: $p = P(Z > 0)$, $p_1' = P(Z + Z' > 0)$, $p_2' = P(Z + Z' > 0, Z + Z'' > 0)$ where Z, Z', Z'' are iid with continuous cdf $L(x)$. Write $V_s = \sum\sum_{i<j} V_{ij} + \sum_{i=1}^{N} V_{ii}$. The number of terms in the first sum is $\begin{pmatrix} N \\ 2 \end{pmatrix}$, and the number of terms in the second sum is N.

$$\phi(z_i, z_i) = \begin{cases} 1, & \text{if } z_i + z_i > 0 \\ 0, & \text{otherwise} \end{cases}$$

Thus, $E(V_{ii}) = P(V_{ii} = 1) = P(Z_i > 0) = p$. For $i < j$, $E(V_{ij}) = P(V_{ij} = 1) = P(Z_i + Z_j > 0) = p_1'$. We have

$$E(V_s) = \sum\sum_{i<j} E(V_{ij}) + \sum_{i=1}^{N} E(V_{ii}) = \begin{pmatrix} N \\ 2 \end{pmatrix} p_1' + Np.$$

We calculate he $Var(V_s)$ only for the special case $N = 3$. If $N = 3$, then $V_s = V_{11} + V_{22} + V_{33} + V_{12} + V_{13} + V_{23}$ and $Var(V_s) = Var(V_{11}) + Var(V_{22})+ Var(V_{33}) + Var(V_{12}) + Var(V_{13})+ Var(V_{23})$ $+2Cov(V_{11}, V_{22})+ 2Cov(V_{11}, V_{33})+ 2Cov(V_{11}, V_{12})+ 2Cov(V_{11}, V_{13})+ 2Cov(V_{11}, V_{23})+ 2Cov(V_{22}, V_{33}) +$ $2Cov(V_{22}, V_{12})+ 2Cov(V_{22}, V_{13})+ 2Cov(V_{22}, V_{23})+ 2Cov(V_{33}, V_{12})+ 2Cov(V_{33}, V_{13}) + 2Cov(V_{33}, V_{23})+$ $2Cov(V_{12}, V_{13})+ 2Cov(V_{12}, V_{23})+ 2Cov(V_{12}, V_{33})$. Note that 6 of the covariances are equal to zero due to independence. V_{11}, V_{22}, V_{33} are identically distributed random variables. So they all have the same variance: $Var(V_{11}) = Var(V_{22}) = Var(V_{33}) = E(V_{11}^2) - [E(V_{11})]^2 = E(V_{11}) - [E(V_{11})]^2$. $E(V_{11}) = P(Z_1 > 0) = p$. So, $Var(V_{11}) = Var(V_{22}) = Var(V_{33}) = p - p^2$. Similarly, V_{12}, V_{13}, V_{23} are identically distributed random variables which have the same variance: $Var)V_{12}) = Var(V_{13}) = Var(V_{23}) = E(V_{12}^2) - [E(V_{12})]^2 = p_1' - (p_1')^2$ because $E(V_{12}) = P(Z_1 + Z_2 > 0) = p_1'$. Note that V_{11} and V_{12} are functions of the same Z. Other covariance terms have this same property. So, $Cov(V_{11}, V_{12}) = Cov(V_{11}, V_{13}) = Cov(V_{22}, V_{12}) = Cov(V_{22}, V_{23}) =$ $Cov(V_{33}, V_{13}) = Cov(V_{33}, V_{23})$, i.e. all six nonzero covariance terms in the first four rows are equal. $Cov(V_{11}, V_{12}) = E(V_{11}V_{12}) - E(V_{11})E(V_{12})$, $E(V_{11}) = P(Z_1 > 0) = p$, $E(V_{12}) = P(Z_1 + z_2 > 0) = p_1'$, $E(V_{11}V_{12}) = P(V_{11} = 1 \text{ and } V_{12} = 1) = P(Z_1 > 0 \text{ and } Z_1 + Z_2 > 0)$. At the end of these notes we will show that $P(Z_1 > 0 \text{ and } Z_1 + Z_2 > 0) = \frac{1}{2}\left(p_1' + p^2\right)$. thus, $Cov(V_{11}, V_{12}) = \frac{1}{2}\left(p_1' + p^2\right) - pp_1'$. Note that V_{12} and V_{13} are functions of the same Z but V_{12} and V_{13} are also functions of a different Z. Since other covariance terms involve random variables with this same feature, we have $Cov(V_{12}, V_{13}) = Cov(V_{12}, V_{23}) = Cov(V_{13}, V_{23}) =$ $E(V_{12}V_{13}) - E(V_{12})E(V_{13})$. $E(V_{12}V_{13}) = P(V_{12} = 1 \text{ and } V_{13} = 1) = P(Z_1 + Z_2 > 0 \text{ and } Z_1 + Z_3 > 0) = p_2'$. $E(V_{12}) = E(V_{13}) = P(Z_1 + Z_2 > 0) = p_1'$. Thus, $Cov(V_{12}, V_{13}) = p_2' - (p_1')^2$. Substituting previous results into the general expression for $Var(V_s)$ gives $Var(V_s) = 3(p - p^2) + 3[p_1' - (p_1')^2]+$ $2\left[6\left[\frac{1}{2}(p_1' + p^2) - pp_1'\right] + 3\left[p_2' - (p_1')^2\right]\right]$. Rearranging terms, we have $Var(V_s) = 3(2)[p_2' - (p_1')^2]3p(1-p)+$ $3[2(p - p_1')^2 + 3p_1'(1 - p_1')]$ which is the same as in the general case with $N = 3$.

9.11 Confidence Limits

In this section, we derive confidence limits for a population median and for the center of symmetry of a continuous non-symmetric distribution.

9.11.1 Population Median

Assumption: $Z_1, Z_2, ..., Z_N$ are iid with continuous cdf $L(s)$ and a unique median θ. Let $Z_{(1)} < Z_{(2)} < \cdots < Z_{(N)}$ denote the ordered observations. Problem: find $i < i$ so that $P_\theta(Z_{(i)} < \theta < Z_{(j)}) = 1-\alpha$ subject to the tail probabilities being equal. That is, $P_\theta(\theta < Z_{(i)}) = P_\theta(Z_{(j)} < \theta)$. Solution: The first equation will be satisfied if $P_\theta(\theta < Z_{(i)}) = P_\theta(Z_{(j)} < \theta) = \frac{\alpha}{2}$. Let us first solve for the integer i so that $P_\theta(\theta < Z_{(i)}) = \frac{\alpha}{2}$. Recall from Theorem 3, part (b), $\theta < Z_{(i)}$ iff $S_N(Z-\theta) \geq N-i+1)$. Thus, $P_\theta(\theta < Z_{(i)}) = P_\theta(S_N(Z-\theta) \geq N-i+1)$. If θ is the true value of the population median, then $S_N(Z-\theta)$ has a binomial distribution with parameters N and $p = 0.5$. Thus, $S_N(Z-\theta)$ is distributed like the null distribution of the sign statistic S_N. This implies $P_\theta(\theta < Z_{(i)}) = P_0(S_N \leq N-i+1)$ where the subscript 0 refers to the null distribution of S_N. It does not mean $\theta = 0$.

Since the null distribution of S_N is symmetric, we have $P_\theta(\theta < Z_{(i)}) = P_0(S_N \leq i-1) = \frac{\alpha}{2}$. Thus, we can use Table G in the text book to find i or, if N is large, use the normal approximation to the null distribution of S_N. Suppose i has been found so that $P_\theta(\theta < Z_{(i)}) = \frac{\alpha}{2}$. Now solve for j so that $P_\theta(\theta > Z_{(j)}) = \frac{\alpha}{2}$. But, $\theta > Z_{(j)}$ iff $S_N(Z-\theta) \leq N-j$. So, $P_\theta(\theta > Z_{(j)}) = P_0(S_N \leq N-j) = \frac{\alpha}{2}$. From the original equation, we see that $i-1 = N-j$ or $j = N-i+1$.

Example: Suppose a sample of $N = 20$ observations is taken from a population of measurements that have a continuous distribution with a unique median θ. We believe that $L(x)$ is not a symmetric distribution. Let $Z_{(1)} < Z_{(2)} < \cdots < Z_{(20)}$ denote the ordered observations. Determine $i < j$ so that $(Z_{(i)}, Z_{(j)})$ gives a 95% confidence limits for θ. Solution: We want $0.025 = P_\theta(\theta < Z_{(i)}) = P(S_N \leq i-1)$ where S_N has a binomial distribution with parameters $N = 10$ and $p = 0.5$. From Table G in the text book, $P(S_N \leq 5) = 0.0207$ and $P(S_N \leq 6) = 0.577$. Take $i-1 = 5$. Then, $i = 6$ and $j = N-(i-1) = 20-5 = 15$. Thus, $(Z_{(6)}, Z_{(15)})$ gives a 95.68% confidence limit for θ.

Example: Same as the previous Example except $N = 100$. Solution: We want $0.025 = P_\theta(\theta < Z_{(i)}) = P(S_N \leq i-1)$. We cannot use Table G for $N > 40$. We use the normal approximation and continuity correction. Since S_N is binomial, $N = 100$ and $p = 0.5$. $E(S_N) = NP = 100(0.5) = 50$ and $Var(S_N) = Np(1-p) = 100(0.5)(0.5) = 25$. $0.025 = P(S_N \leq i-1+0.5) = P(S_N \leq i-0.5) = P\left(Z \leq \frac{i-0.5-50}{5}\right)$. From that we get $\frac{i-50.5}{5} = -1.96$. Solving for i we get $i = 40.7$. Take i to be 40. Then $j = N-(i-1) = 100-39 = 61$.

9.11.2 Center of Symmetry

Assumption: $Z_1, Z_2, ..., Z_N$ are iid with a continuous distribution symmetric about θ. That is, we are assuming that the Z_i follow the shift model $Z \overbrace{=}^{\text{ST}} U + \theta$ where U has a distribution symmetric about zero. Let $A_{(1)} < A_{(2)} < \cdots < A_{(M)}$ denote the ordered averages $\frac{Z_i+Z_j}{2}, i \leq j$ where $M = \binom{N}{2} + N$. Also let $V_s(Z-\theta) =$ the number of pairs $(Z_i, Z_j), i \leq j$ for which $\frac{Z_i+Z_j}{2} > \theta$. Problem: Find $i < j$ so that $P_\theta(A_{(i)} < \theta < A_{(j)}) = 1-\alpha$ subject to the tail probabilities being equal. That is $P_\theta(\theta < A_{(i)}) = P_\theta(A\theta > A_{(j)})$. Solution: The above equation will be satisfied if $P_\theta(\theta < A_{(i)}) = P_\theta(A\theta > A_{(j)}) = \frac{\alpha}{2}$. Let us first solve for the integer i so that $P_\theta(\theta < A_{(i)}) = \frac{\alpha}{2}$. By Theorem 3(page 178 in the text book), $\theta < A_{(i)} \Leftrightarrow V_s(Z-\theta) \geq M-i+1$. Thus, $P_\theta(\theta < A_{(i)}) = P_\theta(V_s(Z-\theta) \geq M-i+1)$. If θ is the true value of the shift parameter θ, then $Z_i - \theta$, $i = 1, 2, ..., N$ has a distribution symmetric about zero. That is $V_s(Z-\theta) \overbrace{=}^{\text{ST}} V_s$ where V_s has the null distribution of the signed rank statistic. Thus, $P_\theta(\theta < A_{(i)}) = P_{H_0}(V_s \geq M-i+1)$. Since the null distribution of V_s is symmetric, we have $P_\theta(\theta < A_{(i)}) = P_0(V_s \leq i-1) = \alpha$. Thus Table H in the text book can be used to find i when N is small and the normal approximation to the null distribution of V_s can be used when N is large. After i is found, j is given by $j = M = i+1$.

Example: Assume that $Z_1, Z_2, ..., Z_N$ are iid with a continuous distribution symmetric about θ. Find $i < j$ so that $(A_{(i)}, A_{(j)})$ is a 95% confidence interval for θ when $N = 20$, and (a) using Table H, (b) using the normal approximation.

Solution to (a): $P_\theta(\theta < V_{(i)}) = P_0(V_s \leq i - 1) = 0.025$. From Table H, $P_0(V_s \leq 52) = 0.0242$, and $P_0(V_s \leq 53) = 0.0266$. Take $i - 1 = 52$. Then $i = 53$.

$$M = \begin{pmatrix} N \\ 2 \end{pmatrix} + N = \begin{pmatrix} 20 \\ 2 \end{pmatrix} + 20 = 210. j = M - i + 1 = 210 - 53 + 1 = 158.$$

Thus, $(A_{(53)}, A_{(158)})$ is a $100[1 - 2(0.0242)] = 95.16\%$ confidence interval for θ. Solution to (b):

$$E_{H_0}(V_s) = \frac{N(N+1)}{4} = \frac{20(21)}{4} = 105.$$

$$\sqrt{Var_{H_0}(V_s)} = \sqrt{\frac{N(N+1)(2N+1)}{24}} = \sqrt{\frac{20(21)(41)}{24}} = 26.79.$$

$$P_\theta(\theta < A_{(i)}) = P_0(V_s \leq i - 1) = P\left(Z \leq \frac{i - 0.5 - 105}{26.79}\right) = 0.025.$$

Then, $\frac{i-0.5-105}{26.79} = -1.96$. From that $i = 52.99$. Use $i = 52$.

$$M = \begin{pmatrix} N \\ 2 \end{pmatrix} + N = \begin{pmatrix} 20 \\ 2 \end{pmatrix} + 20 = 210.$$

Then, $j = M - i + 1 = 210 - 52 + 1 = 159$. Thus $(A_{(52)}, A_{(159)})$ is approximately a 95% confidence interval for θ.

9.12 Homework and Answers

Homework from Chapter 4 in the text book.

2. $S_N \sim b(N, p)$. $H_0 : p0.5$. $H_1 : p = P(Z_i \leq 22)$. $S_n = \#(Z_i \leq 22)$. Test for P_Δ. Then the power. $E(S_N) = Np = (20)(0.9772) = 19.544$. $\sqrt{Var(S_N)} = \sqrt{Npq} = \sqrt{20(0.9772)(0.0228)} = 0.668$. Then,

$$\prod = P(S_N \geq 15) = P\left(\frac{S_N - 19.544}{0.668} \geq \frac{14.5 - 19.544}{0.688}\right) = \Phi(7.56) = 0.9999.$$

7. $\alpha = 0.02$. The power is 0.95, $\Delta = 1, \sigma^2 = 2$. Z = treatment observation minus the control observation. $\Delta = E(Z)$. $H_0 : \Delta = 0$ versus $H_1 : \Delta > 0$. S_N = the number of positive $Z's$. Find N so an $\alpha = 0.02$ test has power of 95% against the alternative $\Delta = 1$ when Z has a normal distribution with $\sigma^2 = 2$. Reject H_0 if $S_N \geq c$. $E_{H_0}(S_N) = \frac{N}{2}$.

$$Var_{H_0}(S_N) = np(1-p) = \frac{N}{4}.0.02 = P_{H_0}(S_N \geq c - 0.5) = P_0\left(\frac{S_N \geq c - 0.5 - \frac{N}{2}}{\frac{N}{2}}\right) = 0.05.$$

$$2.05 = \frac{c - 0.5 - \frac{N}{2}}{\frac{N}{2}} \Rightarrow c = 0.5 + \frac{N}{2} + 2.05\left(\frac{\sqrt{N}}{2}\right),$$

$$0.95 = P_\Delta\left(S_N > 0.5 + \frac{N}{2} + \frac{2.05\sqrt{N}}{2}\right)$$

$$E_\Delta(S_N) = Np = N(0.7611).$$

$$p = P(success) = P(Z_i > 0) = P\left(\frac{Z_i - 1}{\sqrt{2}} > \frac{0 - 1}{\sqrt{2}}\right) = \Phi(-0.71) = 0.7611.$$

$$\sqrt{Var_{\Delta}(S_N)} = \sqrt{Np(1-p)} = 0.43\sqrt{N}.$$

$$0.95 = P_{\Delta}\left(\frac{S_N - 0.7611N}{0.43\sqrt{N}} > \frac{0.5 + \frac{N}{2} + \frac{2.05\sqrt{N}}{2} - 0.7611}{0.43\sqrt{N}}\right).$$

Then,

$$\frac{0.5 + \frac{N}{2} + \frac{2.05\sqrt{N}}{2} - 0.7611N}{0.43\sqrt{N}} = 1.645.$$

Thus, $N = 44$.

10.i Z_i = after minus before. $H_0 : \Delta = 0$. $H_1 : \Delta > 0$. $\Delta = E(Z_i)$. V_s = sum of ranks of z_i. $\alpha = 0.0527$ level test. $N = 10$. Reject H_0 if $V_s \geq 44$. The power

$$\frac{\Delta}{\tau} = 0.5 = P_{\Delta}(V_s \geq 44).$$

Find $E_{\Delta}(V_s)$ and approximate $E_{\Delta}(V_s) = E_{H_0}(V_s)$. The answer might not match 0.3861.

$$\sqrt{Var_{\Delta}(V_s)} = \sqrt{Var_0(V_s)} = \sqrt{\frac{N(N+1)(2N+1)}{24}} = \sqrt{\frac{10(11)(21)}{24}} = 9.8107.$$

$$E_{\Delta}(V_s) = \begin{pmatrix} N \\ 2 \end{pmatrix} p_1' + Np.$$

$\sigma = 2$ and $\frac{\Delta}{\sigma} = 0.5$. Then, $\Delta = 1$. So,

$$E_{\Delta}(V_s) = \begin{pmatrix} 10 \\ 2 \end{pmatrix} \frac{1}{2} + 10p.$$

$$p = P_{\Delta}(Z_i > 0) = P\left(\frac{z_i - 1}{2} > \frac{0-1}{2}\right) = P(W > -0.5) = 1 - \Phi(0.5) = 0.6915.$$

$$p_1' = P_{\Delta}(Z_i + Z_j > 0) \sim N(2\Delta, 2\sigma^2).$$

$$P_{\Delta}\left(\frac{z_i + z_j - 2}{2.8284} > \frac{0-2}{2.8284}\right) = 0.7611 = P(W > -0.71).$$

$$E_{\Delta}(V_s) = 45(0.7611) + 10(0.6915) = 41.1645.$$

$$\prod_{\Delta} = P(V_s \geq 44) = P\left(\frac{V_s - 41.16}{9.8107} \geq \frac{44 - 41.16}{9.8107}\right) = P(Z \geq 0.286) = 1 - 0.6141 = 0.6141.$$

11.ii $\alpha = 0.97, \sigma = 2, N = 10$. $\frac{\Delta}{\tau} = 0.75 \Rightarrow \frac{\Delta}{2} = 0.75 \Rightarrow \Delta = 1.5$.

$$\sqrt{Var_{\Delta}(V_s)} = \sqrt{V_{H_0}(V_s)} = \sqrt{\frac{N(N+1)(2N+1)}{24}} = \sqrt{\frac{10(11)(21)}{24}} = 9.8107.$$

$$p = P_{\Delta}(Z_i > 0) = P\left(\frac{z_i - 1.5}{2} > \frac{0-1.5}{2}\right) = P(w > -0.75) = 0.7734.$$

$$p_1' = P_{\Delta}(z_i + z_j > 0) \sim N(2\Delta, 2\sigma^2).$$

$$P_{\Delta}\left(\frac{z_i + z_j - 3}{2.8284} > \frac{0-3}{2.8284}\right) = P_{\Delta}(W > -1.061) = \Phi(1.061) = 0.8554.$$

$$E_{\Delta}(V_s) = \begin{pmatrix} N \\ 2 \end{pmatrix} p_1' + Np =$$

$$M = \begin{pmatrix} 10 \\ 2 \end{pmatrix} 0.8554 + 10(0.7734) = 46.227.$$

From the tables, it can be concluded that we reject when $V_s \geq 41$. The power then is

$$P_{\Delta}(V_s \geq 41) = P_{\Delta}(V_s \geq 41 - 0.5) = P_{\Delta}\left(Z \geq \frac{40.5 - 46.227}{9.8107}\right) = \Phi(0.58) = 0.7190.$$

12.ii z = taped minus sutured. $\Delta = E(Z_i)$. $H_0 : \Delta = 0$. $H_1 : \Delta > 0$. $\alpha = 0.02$, $N = 25$. Reject H_0 if $V_s \geq c$. Power($\Delta = 10$), Z normal, $\tau = 15 = \sigma$.

$$E_{H_0}(V_s) = \frac{N(N+1)}{4} = \frac{25(26)}{4} = 162.5$$

$$\sqrt{Var_{H_0}(V_s)} = \sqrt{\frac{N(N+1)(2N+1)}{24}} = \sqrt{\frac{25(26)(51)}{24}} = 37.165. P\left(z \geq \frac{c - 162.5 + 0.5}{37.165}\right) = 0.02.$$

Then, $\frac{c-162.5+0.5}{37.165} = 2.054 \Rightarrow c = 238.34 \Rightarrow c = 239$. Find $P_\Delta(V_s \geq 239)$.

$$E_\Delta(V_s) = \binom{25}{2} p_1' + Np.$$

$$p = P_\Delta(Z_i > 0) = P\left(\frac{z_i - 10}{15} > \frac{0-10}{15}\right) = P(W > -0.67) = \Phi(0.67) = 0.7486.$$

$$p_1' = P_\Delta(z_i + z_j > 0) = P\left(W > \frac{0-20}{\sqrt{450}}\right) = P(W > -0.94) = 0.8264.$$

Then, $E_\Delta(V_s) = \binom{25}{2} 0.8264 + 25(0.7486) = 266.64$. The power is

$$P\left(Z \geq \frac{239 - 266.64}{37.165}\right) = P(Z \geq -0.74) = 0.7704.$$

22. Determine $\hat{\theta} = median(z_i)$, and $\bar{\theta} = \frac{\sum z_i}{N}$. $\hat{\theta} = median(A_i)$; $N = 12$. $z_i = -0.11, -0.05, 0.01, 0.14, 0.15, 0.15, 0.37, 0.44, 0.69, 0.75, 0.98, 1.19$. $\tilde{\theta}$ = average of the two middle values $= \frac{0.15+0.37}{2} = 0.26$. $\bar{\theta} = \frac{\sum z_i}{N} = \frac{4.71}{12} = 0.393$. $\hat{\theta} = \#$ of pairs $(z_i, z_j), i \leq j$. There are $m = 78$ values $A_1, ..., A_{78}$. $\hat{\theta}$ = average of the two middle values $\frac{A_{(39)}+A_{(40)}}{2} = \frac{0.37+0.38}{2} = 0.375$.

29.iii $N = 19$, $\alpha = 0.95$. Find $i < j$ such that $P_\theta(A_i < \theta < A_j) = 0.95$. Want $0.025 = P_{H_0}(V_s \leq i-1)$. From Table H, $P(V_s \leq 46) = 0.0247$. $i - 1 = 46 \rightarrow i = 47$. Then, $j = N - i + 1 = 190 - 46 = 144$. The confidence is 95.06%.

30.iii Find a 95% confidence interval. $N = 19$. $P(\mu \leq z_i) = P_0(S_N \leq i-1) = 0.025$. $P_0(S_N \leq 5) = 0.0096$. Take $i - 1 = 4$. Then, $i = 5$. $j = N + 1 - i = 19 + 1 - 5 = 15$. (z_5, z_{15}) is the confidence interval.

31 $N = 12$, z_i = after minus before. Part (a): Find $i < j$ so that $P_\theta(\theta < z_i) = P(S_N \leq i-1)$. In Table G of the text book, $P(S_N \leq 2) = 0.0193 \Rightarrow i - 1 = 2 \Rightarrow i = 3$. $j = N - i + 1 = 12 - 2 = 10$. (z_3, z_{10}) gives a 95% confidence interval. $z_3 = 0.01$, and $z_{10} = 0.75$. Then, $(0.01, 0.75)$ is a specific 95% confidence interval for θ.

Part (b): Find $i < j$ so that $P_\theta(A_i < \theta < A_j) = 0.95$. $0.025 = P_\theta(\theta < A_i) = P_{H_0}(V_s \leq i-1)$. From table H in the text book, $P_{H_0}(V_s \leq 13) = 0.0212$. Then, $i - 1 = 13 \Rightarrow i = 14$. $j = m - i + 1 \Rightarrow j = 78 - 13 = 65$. (A_{14}, A_{65}) gives a 95% confidence interval. $A_{14} = 0.08$, and $A_{65} = 0.53 \Rightarrow (0.08, 0.53)$.

Part (c): $t_0 = 2.201$, $\bar{\theta} = 0.393$. $\bar{\theta} \pm t_0 \frac{s}{\sqrt{n}}$. $s = 0.4239$. $0.393 \pm 2.201 \left(\frac{0.4239}{\sqrt{12}}\right) = (0.124, 0.662)$.

33.i $1 - \alpha = 0.95$. $N = 25$. $P_\theta(\theta \leq A_i) = P_{H_0}(V_s \leq i-1) = 0.025$. $E_{H_0}(V_s) = \frac{N(N+1)}{4} = \frac{25(26)}{4} = 162.5$. $\sqrt{Var_{H_0}(V_s)} = \sqrt{\frac{N(N+1)(2N+1)}{24}} = \sqrt{\frac{25(26)(51)}{24}} = 37.165$.

$$P_{H_0}\left(Z \leq \frac{i - 1 + 0.5 - 162.5}{37.165}\right) = 0.025.$$

Then, $\frac{i-0.5-162.5}{37.165} = -1.96 \Rightarrow i = 90.16 \Rightarrow i = 90$. $M = \begin{pmatrix} 25 \\ 2 \end{pmatrix} + 25 = 325$. $j = M - i + 1 \Rightarrow j = 325 - 90 + 1 = 236$.

34.i $P(\mu < z_i) = P(S_N \leq i - 1) \Rightarrow S_N = 7$. $P(S_N \leq 5) = 0.02$. $i - 1 = 7 \Rightarrow i = 8$. $j = N - i + 1 = 25 - 8 + 1 = 18$.

63.i Reject when $V_s \geq c$. $V_s(z) = \sum\sum_{i\leq j} \phi(z_i, z_j)$. $z_i, z_{i'} \in \{1, 2, ..., N\}$ and $z_i < z_{i'}, \forall i$. Then, $\sum\sum_{i\leq j} \phi(z_i, z_j) \leq \sum\sum_{i\leq j} \phi(z_{i'}, z_{j'}) \forall i, j$ because $\phi(u, v)$ sums positive numbers and will not get smaller on each iteration. Then, it is true that $V_s(z) \leq V_s(z')$. If we reject when $V_s(z) \geq c$, then we will reject on $V_s(z')$ also. $V_s(z') \geq V_s(z) \geq c$.

9.13 Comparison of More Than Two Treatments

This section does not discuss paired data.

Example: Brands A, B, C of tranquilizers are to be compared in terms of which brand, if any, most improves the health of mental patients of $N = 7$ patients, 2 are randomly assigned to brand A, and 3 to brand B, and 2 to brand C. After a 1-month period, the $N = 7$ patients are ranked according to improvement. The results are:

Treatment	Combined Rank
A	2,4
B	3,5,7
C	1,6

H_0 : No difference in improvement among the 3 brands versus H_1 : 2 or more brands differ with respect to improvement In the randomization model, under H_0 each of the outcomes is equally likely. That is, the rankings we observe are due to chance assignment of the subjects to the three groups. The number of possible outcomes is equal to the number of ways of assigning 2 subjects to treatment A, 3 to B, and 2 to C. $\frac{7!}{2!3!2!} = 210$. In general, if there are s treatment groups and if $n_1, n_2, ..., n_s$ subjects are randomly assigned to each of these groups with a total of $N = n_1 + n_2 + \cdots + n_s$ subjects, then the total number of possible outcomes is $\frac{N!}{n_1!n_2!\cdots n_s!}$. The general layout of the data in the comparison of s groups is

Trt	1	2	3	$\cdots$	s
	x_{11}	x_{21}	x_{31}	...	x_{s1}
	x_{12}	x_{22}	x_{32}	...	x_{s2}
	.	.	.	...	.
	.	.	.	...	.
	.	.	.	...	.
	x_{1n_1}	x_{2n_2}	x_{3n_3}	...	x_{sn_s}

The layout of the ranks is

Trt	1	2	3	$\cdots$	s
	R_{11}	R_{21}	R_{31}	...	R_{s1}
	R_{12}	R_{22}	R_{32}	...	R_{s2}
	.	.	.	...	.
	.	.	.	...	.
	.	.	.	...	.
	R_{1n_1}	R_{2n_2}	R_{3n_3}	...	R_{sn_s}
Sums	R_1	R_2	R_3	...	R_s

The average ranks are denoted by $\bar{R}_1.$, $\bar{R}_2.$, $\bar{R}_3.$, ... $\bar{R}_s.$ where $R_1. = \frac{\sum R_{1i}}{n_1}$, *etc.* The sum of all the ranks is $\frac{N(N+1)}{2}$. the overall average rank is $\bar{R}$... The number of possible outcomes is $\frac{N!}{n_1!n_2!\cdots n_s!}$.

9.13.1 Kruskal-Wallis Test

H_0 : no treatment effect. Under H_0, $R_i.$ should tend to fall close to R... This suggests

$$k = \frac{12}{N(N+1)} \sum_{i=1}^{s} n_i \left(R_i. - \frac{N+1}{2} \right)^2 .$$

Another expression for K is

$$K = \frac{12}{N(N+1)} \sum_{i=1}^{s} \frac{R_i^2}{n_i} - 3(N+1).$$

proof:

$$\sum_{i=1}^{s} n_i \left(R_i. - \frac{N+1}{2} \right)^2 = \sum_{i=1}^{s} n_i \left(R_{i.}^2 - 2R_i.\frac{N+1}{2} + \frac{(N+1)^2}{4} \right) =$$

$$\sum n_i R_{i.}^2 - (N+1) \sum R_i.n_i + \frac{(N+1)^2}{4} \sum n_i = \sum n_i \left(\frac{R_i.}{n_i} \right)^2 - (N+1) \sum R_i + \frac{(N+1)^2}{4} N =$$

$$\sum n_i \left(\frac{R_i.}{ni} \right)^2 - \frac{(N+1)^2 N}{2} + \frac{(N+1)^2 N}{4} = \sum \frac{R_{i.}^2}{n_i} - \frac{N(N+1)^2}{4}.$$

$$K = \left(\frac{12}{N(N+1)} \sum \frac{R_{i.}^2}{n_i} \right) - 3(N+1).$$

Example: $N = 7$. $R_1. = 6$, $R_2. = 15$, $R_3. = 7$. $n_1 = 2, n_2 = 3, n_3 = 2$. Then,

$$K = \frac{12}{7(8)} \left(\frac{6^2}{2} + \frac{15^2}{3} + \frac{7^2}{2} \right) - 3(8) = 1.18.$$

The null distribution of K can be determined by enumerating all possible ways of assigning 2 ranks to A, 3 to B, and 2 to C. $\frac{7!}{2!3!2!} = 210$. Table I in the text book gives Kruskal-Wallis statistics for small s. $P_{H_0}(K \geq c)$ is given for $s = 3$ and all combinations of (n_1, n_2, n_3) when $n_i \leq 5$. Our example corresponds to $s = 3$, $n_1 = 2, n_2 = 3, n_3 = 2$(any order will work). For $s = 3$ and $n_i > 5, i = 1, 2, 3$ or when $s > 3$ and $n_i > 4$, it is claimed that the null distribution of K is approximately Chi-square with $s-1$ degrees of freedom.

Example: Page 207 in the text book. The data is

Size	Diet	Growth
$n_1 = 8$	A_1	164,190,203,205,206,214,228,257
$n_2 = 4$	A_2	185,197,201,231
$n_3 = 7$	A_3	187,212,215,220,248,265,281
$n_4 = 6$	A_4	202,204,207,227,230,276

The ordered ranks in tabular form are:

Size	Diet	Growth
$n_1 = 8$	A_1	1,4,8,10,11,14,18,22
$n_2 = 4$	A_2	2,5,6,20
$n_3 = 7$	A_3	3,13,15,16,21,23,25
$n_4 = 6$	A_4	7,9,12,17,19,24

i	R_i	R_i^2	n_i	$\frac{R_i^2}{n_i}$
1	88	7744	8	968
2	33	1089	4	272.25
3	116	13456	7	1922.29
4	88	7744	6	1290.67

$\sum_{i=1}^{4} \frac{R_i^2}{n_i} = 4453.21$. Thus, $K = \frac{12}{25(26)}(4453.21) - 3(26) = 4.21$. Reject H_0 if $K \geq c$. p-value $= \hat{\alpha} = P_{H_0}(K \geq 4.21) = P(\chi^2(3) \geq 4.21) = 0.2241 < \hat{\alpha} < 0.2407$. If $\alpha = 0.05$, then what is c? $c = 8.00$, $\hat{\alpha} = 0.0460$.

If $s = 2$, then the Kruskal-Wallis test is equivalent to a 2-tailed test based on the Wilcoxon rank sum test. Use the rank sum statistic $W_s = R_2$. Under the shift model $\Delta = E(y - x)$. $H_0 : \Delta = 0$. $H_1 : \Delta \neq 0$. Reject H_0 if $W_s \leq c_1$ or $W_s \geq c_2$. Find c_1 and c_2. $E_{H_0}(W_s) = \frac{n(N+1)}{2}$. Then, $c_1 = \frac{n(N+1)}{2} - c$ and $c_2 = \frac{n(N+1)}{2} + c$. Reject H_0 if $|W_s - E_{H_0}(W_s)| \geq c$ or $W_s - \frac{n(N+1)}{2} \geq c$ or $W_s - \frac{n(N+1)}{2} \leq -c$. Claim that the above is the same as the Kruskal-Wallis statistic. The proof is omitted.

9.13.2 Tied Observations

In the case of tied observations, we form the combined set and assign midranks. N is the total number of observations. e is the number of distinct values. d_1 is the number of observations tied at the smallest value. d_2 is the number of observations tied at the next largest value and so on... $d_1 + d_2 + \cdots + d_e = N$. R_i^* is the sum of the midranks of the observations in group i. K^* is the Kruskal-Wallis midrank statistic.

$$K^* = \frac{\frac{12}{N(N+1)} \sum_{i=1}^{s} \frac{R_{i.}^{*2}}{n_i} - 3(N+1)}{1 - \sum_{i=1}^{e} \frac{d_i(d_i-1)^2}{N^3 - N}}.$$

Reject H_0 when $K^* \geq c$. The null distribution of K^* can be approximated when n_i is large by a Chi-square distribution with $s - 1$ degrees of freedom.

Example: Comparison of 4 labs(page 209 of the text book).

Lab	
A	38.7,41.5,43.8,44.5,45.5,46.47.7,58
B	39.2,39.3,39.7,41.4,41.8,42.9,43.3,45.8
C	34,35,39,40,43,43,44,45
D	34,34.8,34.8,35.4,37.2,37.8,41.2,42.8

The midranks of each lab are

Lab	n_i	R_i^*
A	8	197
B	8	142
C	8	125.5
D	8	63.5

$\frac{\sum R_i^{*2}}{n_i} = 9844.44$. The numerator of K^* is $\frac{12}{32(33)}(9844.44)-3(33) = 12.87$. All the $d_i = 1$ except $d_1 = 2, d_2 = 2$ and some other $d_i = 2$. The denominator of K^* is $1 - \frac{2(2^2-1)+2(2^2-1)+2(2^2-1)}{32^3-32} = 0.99945$. $K^* = \frac{12.87}{0.99945}12.88$ $\hat{\alpha} = P_{H_0}(K^* \geq 12.87) = P(\chi^2(3) \geq 12.87) = 0.0059$. Reject H_0.

9.13.3 $2 \times t$ Contingency Tables

Example: # 4 on page 210 of the text book.

	A	B	C	D	F	
Live	3	8	25	10	4	50
TV	10	18	12	8	2	50
	13	26	37	18	6	100

$N = 100$. The Kruskal-Wallis statistic cannot be used for a 1-sided test. It only tests 2-sided alternatives.

Example: Page 306 in the text book.

	Level of Suffering				
	Severe	Moderate	Slight	None	
Placebo	8	8	19	35	70
Drug P	2	3	5	20	30
Drug C	3	4	15	45	67
	13	15	39	100	167
	d_1	d_2	d_3	d_4	

$e = 4$. H_0 : No treatment effects. H_1 : The 3 groups differ. Midrank of severe is $\frac{d_1+1}{2} = 7$. Midrank of moderate is $d_1 + \frac{d_2+1}{2} = 13 + \frac{16}{2} = 21$. Midrank of slight is $d_1 + d_2 + \frac{d_3+1}{2} = 13 + 15 + \frac{40}{2} = 48$. Midrank of none is $d_1 + d_2 + d_3 + \frac{d_4+1}{2} = 13 + 15 + 39 + \frac{101}{2} = 117.5$ $R_1^* = 8(7) + 8(21) + 19(48) + 35(100) = 5248.5$. $R_2^* = 2667; R_3^* = 6112.5$. $N = 167$. $K^* = 5.5009$. $\hat{\alpha} = P_0(K^* \geq 5.5009) = P(\chi^2(2) \geq 5.5009) = 0.0672$.

Example: Page 218, example 7.

Response	Y	B	W	C	
Returned	73	65	60	54	252
Not returned	71	76	87	86	320
	144	141	147	140	572

Note: there are only 2 categories. H_0 : Card color has no effect on return rate. H_1 : It does have an effect. Midrank of returns: $\frac{d_1+1}{2} = \frac{252+1}{2} = 126.5$. Midrank of not returned: $d_1 + \frac{d_2+1}{2} = 252 + \frac{320+1}{2} = 412.5$. $R_1^* = 73(126.5) + 71(412.5) = 28522$. $R_2^* = 65(126.5) + 76(412.5) = 39572.5$. $R_3^* = 43477.5; R_4^* = 42306$. $\frac{\sum R_i^{*2}}{n_i} = 47054836$. $K^* = 5.14$. The example on page 212 is very similar.

9.13.4 Multiple Comparisons

Suppose we test a series of 6 hypotheses concerning the 4 labs. H_{10} : Labs 1 and 2 do not differ. H_{20} : Labs 1 and 3 do not differ. ... H_{60} : Labs 5 and 6 do not differ. Suppose each of the 6 tests is performed using the same Type I error rate α. The α is called the *per comparison error rate.* Let F_i be the event that hypothesis H_{i0} is rejected. Then, $\alpha = P_{H_0}(E_i), i = 1, 2, ..., 6$. The experiment wise, or overall Type I error rate, denoted by α' is $\alpha' = P_{H_0}(E_1 \cup E_2 \cup \cdots \cup E_6)$. Since $P_{H_0}(E_1 \cup E_2 \cup \cdots \cup E_6) \leq P_{H_0}(E_1) + P_{H_0}(E_2) + \cdots$, we have $\hat{\alpha} = 6\alpha$. Thus we can force the overall Type I error rate to be small by taking the per comparison error rate to be equal to some small value. For example, if the overall Type I error rate is specified to be $\hat{\alpha} = 0.06$, then we take $\alpha = \frac{\hat{\alpha}}{6} = 0.01$. In general, in comparing s treatments there are $\frac{s(s-1)}{2}$ possible pairwise comparisons. So, for a given $\hat{\alpha}$, we could take the per comparison error rate to be $\alpha = \frac{2\hat{\alpha}}{s(s-1)}$. We will not do this. We will just take α to be some small value such as $\alpha = 0.01$. Forcing α to be quite small will increase the probability of making a Type II error and we become less likely to detect treatment differences.

We study a multiple comparison procedure based on *pairwise rankings.* To compare treatment i and treatment j, we form the combined set of $n_i + n_j$ observations in these 2 groups. Let $R_i^{(j)}$ be the sum of the ranks of the treatment i observations in the combined ranking of all observations in groups i and j only. Then, $R_i^{(j)}$ is the Wilcoxon rank sum statistic studied earlier. $E_{H_0}(R_i^{(j)}) = \frac{n_i(n_i+n_j+1)}{2}$, $Var_{H_0}(R_i^{(j)}) = \frac{n_i n_j(n_i+n_j+1)}{12}$. The decision rule for a 2-sided test: Treatments i and j differ if $R_i^{(j)} \leq c_1$ or if $R_i^{(j)} \geq c_2$. Table B in the text book can be used if there are no ties. Another form of the decision rule: Treatments i and j differ if $|R_i^{(j)} - E_{H_0}(R_i^{(j)})| \geq z_{\alpha/2}\sqrt{Var_{H_0}(R_i^{(j)})}$. This form is convenient when we are using the normal approximation. If there are ties, we must use the normal approximation with the following null mean and variance: $E_{H_0}(R_i^{8(j)}) = \frac{n_i(n_i+n_j+1)}{2}$, $Var_{H_0}(R_i^{*(j)}) = \frac{n_i n_j(n_i+n_j+1)}{12} - \frac{n_i n_j \sum_{i=1}^{e} d_i(d_i^2-1)}{12N(N-1)}$. Notes:

- If there are few ties, then the second term in the variance is small.
- When making pairwise comparisons with contingency table data, we cannot ignore the correction for ties.
- If ties are present and if $Var_{H_0}(R_i^{*(j)})$ is approximated by $Var_{H_0}(R_i^{(j)})$, then

$$\alpha = P_{H_0}\left(\left|R_i^{*(j)} - E_{H_0}(R_i^{*(j)})\right| \geq z_{\alpha/2}\sqrt{Var_{H_0}(R_i^{*(j)})}\right) \geq$$

$$P_{H_0}\left(\left|R_i^{*(j)} - E_{H_0}(R_i^{*(j)})\right| \geq z_{\alpha/2}\sqrt{Var_{H_0}(R_i^{(j)})}\right).$$

  Thus, the actual per comparing error rate as given by the right hand term does not exceed the specified per comparison error rate, α.

Example: Page 240 of the text book. Comparison of 4 labs. Recall, for the Kruskal-Wallis test, the significance probability was $P_{H_0}(D^* \geq 12.88) = 0.0059$.

AB: 38.7(1), 39.2(2), 39.3(3), 39.7(4), 41.4(5), 41.5(6), 41.8(7), 42.9(8) 43.3(9), 43.8(10), 44.5(11), 45.5(12), 45.8(13), 46.0(14), 47.7(15), 58.0(16). $R_A^{*(B)} = 1+6+10+11+12+14+15+16 = 85$ = sum of the lab A ranks.

AC: 34.0(1), 35.0(2), 38.7(3), 39.0(4), 40.0(5), 41.5(6), 43.0(7.5), 43.0(7.5), 43.8(9), 44.0(10), 44.5(11), 45.0(12), 45.5(13), 46.0(14), 47.7(15), 58.0(16). $R_A^{*(C)} = 3 + 6 + 9 + 11 + 13 + 14 + 15 + 16 = 87 =$ sum of the lab A midranks.

AD: 34.0(1), 34.8(2.5), 34.8(2.5), 35.4(4), 37.2(5), 37.8(6), 38.7(7), 41.2(8), 41.5(9), 42.8(10), 43.8(11), 44.5(12), 45.5(13), 46.0(14), 47.7(15), 58.0(16). $R_A^{*(D)} = 7 + 9 + 11 + 12 + 13 + 14 + 15 + 16 = 97 =$

sum of lab A midranks.

BC: 34.0(1), 35.0(2), 39.0(3), 39.2(4), 39.3(5), 39.7(6), 40.0(7), 41.4(8), 41.8(9), 42.9(10), 43.0(11.5), 43.0(11.5), 43.3(13), 44.0(14), 45.0(15), 45.8(16). $R_B^{*(C)} = 4+5+6+8+9+10+13+16 = 71 =$ sum of the lab B midranks.

BD: 34.0(1), 34.8(2.5), 34.8(2.5), 35.4(4), 37.2(5), 37.8(6), 39.2(7), 39.3(8), 39.7(9), 41.2(10), 41.4(11), 41.8(12), 42.8(13), 42.9(14), 43.3(15), 45.8(16). $R_B^{*(D)} = 7 + 8 + 9 + 11 + 12 + 14 + 15 + 16 = 92 =$ sum of the lab B midranks.

CD: 34.0(1.5), 34.0(1.5), 34.8(3.5), 34.8(3.5), 35.0(5), 35.4(6), 37.2(7), 37.8(8), 39.0(9), 40.0(10), 41.2(11), 42.8(12), 43.0(13.5), 43.0(13.5), 44.0(15), 45.0(16). $R_C^{*(D)} = 5+9+10+13.5+13.5+15+16 = 83.5 =$ sum of lab C midranks.

Summary:

Comparison	$R_i^{*(j)}$	$E_{H_0}(R_i^{*(j)})$	$\sqrt{Var_{H_0}(R_i^{(j)})}$
A vs B	85	68	9.52
A vs C	87	68	9.52
A vs D	97	68	9.52
B vs C	71	68	9.52
B vs D	92	68	9.52
C vs D	83.5	68	9.52

$E_{H_0}(R_i^{*(j)}) = \frac{n_i(n_i+n_j+1)}{2} = \frac{8(17)}{2} = 68$. $\sqrt{Var_{H_0}(R_i^{*(j)})} = \sqrt{\frac{n_in_j(n_in_j+1)}{12}} = \sqrt{\frac{8(8)(17)}{12}} = 9.52$. Use a per comparison error rate of $\alpha = 0.02$. The decision rule is labs i and j differ if $|R_i^{*(j)} - E_{H_o}(R_i^{*(j)})| \geq z_{\alpha/2}\sqrt{Var_{H_0}(R_i^{(j)})} = 2.33(9.52) = 22.18$. Conclusions: $|R_A^{*(B)} - 68| = 17$. $|R_A^{*(C)} - 68| = 19$. $|R_A^{*(D)} - 68| = 29$. $|R_B^{*(C)} - 68| = 3$. $|R_B^{*(D)} - 68| = 24$. $|R_C^{*(D)} - 68| = 15.5$. Therefore, A and D differ, B and D differ at an overall significance level α' not exceeding $6(0.02) = 0.12$.

9.13.5 One-sided Procedures

This section deals with one-sided procedures for comparing several treatments with a control. We have already discussed the example on page 228 of the text book in which we compared several treatments with a control. The same problem may arise when the data is in the form of a contingency table. Consider again the example on page 306 of the text book.

Treatment	Severe	Moderate	Slight	None	Row Totals
Placebo(1)	8	8	19	35	70
Drug P(2)	2	3	5	20	30
Drug C(3)	3	4	15	45	67
Column Totals	15	15	39	100	167

Determine which of the drugs provide a significant improvement over the control using an error rate per comparison of $\alpha = 0.05$ and a pairwise ranking procedure. Solution: pair wise ranking of observations in rows (1) and (2). H_0 : No difference. H_1 : (2) is superior to (1).

Treatment	Severe	Moderate	Slight	None	Row Totals
(1)	8	8	19	35	70
(2)	2	3	5	20	30
Column Totals	10	11	24	55	100

The response categories are ordered as follow: Severe(1), Moderate(2), Slight(3), None(4). Note: higher values imply greater improvement.

Midrank of Severe: $\frac{d_1+1}{2} = \frac{10+1}{2} = 5.5$. Midrank of Moderate: $d_1 + \frac{d_2+1}{2} = 10 + \frac{11+1}{2} = 16$. Midrank of Slight $d_1 + d_2 + \frac{d_3+1}{2} = 10 + 11 + \frac{24+1}{2} = 33.5$. Midrank of None: $d_1 + d_2 + d_3 + \frac{d_4+1}{2} = 10 + 11 + 24 + \frac{55+1}{2} = 73$. $R_2^{*(1)}$ = sum of treatment (2) midranks in a pairwise ranking of the observations under treatments (1) and (2) $= 2(5.5) + 3(16) + 5(33.5) + 20(73) = 1686.5$.

Pairwise ranking of the observations in rows (1) and (3):

Treatment	Severe	Moderate	Slight	None	Row Totals
(1)	8	8	19	35	70
(3)	3	4	15	45	67
Column Totals	11	12	34	80	137

Midrank of Severe: $\frac{d_1+1}{2} = \frac{11+1}{2} = 6$. Midrank of Moderate: $d_1 + \frac{d_2+1}{2} = 11 + \frac{12+1}{2} = 17.5$ Midrank of Slight $d_1 + d_2 + \frac{d_3+1}{2} = 11 + 12 + \frac{34+1}{2} = 40.5$ Midrank of None: $d_1 + d_2 + d_3 + \frac{d_4+1}{2} = 11 + 12 + 34 + \frac{80+1}{2} = 97.5$ $R_3^{*(1)}$ = sum of treatment (3) midranks in a pairwise ranking of observations under treatment (1) and (2) $= 3(6) + 4(17.5) + 15(40.5) + 45(97.5) = 5083$.

Comparison of treatments (1) and (2): note $n = n_2, m+n_1, N = n_1+n_2$. $E_{H_0}(R_2^{*(1)}) = \frac{n(N+1)}{2} = \frac{30(100+1)}{2} = 1515$. $Var_{H_0}(R_2^{*(1)}) = \frac{mn(N+1)}{12} - \frac{mn\sum(d_i^3-d_i)}{12N(N-1)} = 14450.2$. $\sqrt{Var_{H_0}(R_2^{*(1)})} = 120.2$. If treatment (2) is superior to treatment (1), then the observations under treatment (2) should tend to have the higher ranks. Thus we reject H_0 if $R_2^{*(1)} \geq c$. The significance probability is $P_{H_0}(R_2^{*(1)} \geq 1686.5) =$

$$P\left(Z \geq \frac{1686.5 - 1515}{120.2}\right) = P(Z \geq 1.43) = 0.0764.$$

Since the significance probability is greater than 0.05, treatments (1) and (2) are not significantly different. Comparison of (3) and (1): note $n = n_3, m = n_1, N = n_1 + n_3$. $E_{H_0}(R_3^{*(1)}) = \frac{n(N+1)}{2} = \frac{67(137+1)}{2} = 4623$. $\sum d_i(d_i^2-1) = 11^3 + 12^3 + 34^3 + 80^3 - [11+12+34+80] = 554226$. $Var_{H_0}(R_3^{*(1)}) = \frac{mn(N+1)}{12} - \frac{mn\sum(d_i^3-d_i)}{12N(N-1)} = \frac{70(67)(137+1)}{12} - \frac{70(67)(554226)}{12(137)(136)} = 42309.3$. $\sqrt{Var_{H_0}(R_3^{*(1)})} = 205.7$. Since treatment (3) being superior to treatment (1) implies the observations under treatment (3) should tend to have higher ranks, we reject H_0 if $R_3^{*(1)} \geq c$. The significance probability is $P_{H_0}(R_3^{*(1)} \geq 5083) =$

$$P\left(Z \geq \frac{5083 - 4623}{205.7}\right) = P(Z \geq 3.99) < 0.0002 < 0.05.$$

So, treatment (3) is superior to treatment (1) at significance level $\alpha = 0.05$

Chapter 10

SAS Programming

Dr. Morgan, Old Dominion University
Statistics 505, Fall 1996
Text used: Quick Start to Data Analysis with SAS, DiIorio, Frank C., and Kenneth A. Harding.

10.1 SAS Data Sets

When creating a SAS data set, you are specifying what the raw data means. SAS names are:

1. 1–8 characters long.
2. Can include numbers and letters.
3. Can include underscores.

Data sets end with "RUN;" PROC steps perform analysis on a data set. Every SAS job has 2 steps:

1. Data Set.
2. PROC steps.

Every line in SAS ends with a semicolon. "LABEL" means to associate the variable name with human readable text. SAS is not case sensitive. The "SET CASE MIXED" MVS command allows you to edit in lower case on the mainframe. Every data set has a name. Dots in raw data mean information is missing. The "INFILE" statement tells SAS where to find the file. The "INPUT" statement lists the variable names in the "INFILE" statement file name. If no columns are specified, a blank is assumed to separate the data.

```
* ASSIGNMENT 1;
EDIT THE FILE YOU CREATED IN THE FIRST CLASS TO INCLUDE THE
CHANGES BELOW. RUN THIS JOB, THEN BRING THE OUTPUT FOR BOTH
VERSIONS TO THE NEXT CLASS. NOTE: BE CAREFUL TO DISTINGUISH
BETWEEN "ONES" AND "ELLS".;

* SIMPLE PROGRAM TO DEMONSTRATE SAS'S LOOK AND FEEL;

OPTIONS NODATE LINESIZE=72;

DATA STATES;
INFILE 'STATES1 RAW A';
INPUT NAME $ 4-19 HIGHTEMP 25-27 LOWTEMP 29-31
      POP80 POPSQMI FARMPCT PCTURB
```

```
       @83 PCAPINC 5.;
URB_POP = (PCTURB * POP80) / 100;
TEMPRNGE = HIGHTEMP - LOWTEMP;
IF  ((FARMPCT>50)&(PCAPINC>7000)) THEN RICHFARM = 'YES';
ELSE RICHFARM = 'NO';

FORMAT POP80 URB_POP COMMA11. FARMPCT PCTURB 6.2 PCAPINC DOLLAR8.;
LABEL NAME = 'State name"
      HIGHTEMP = 'Highest recorded temperature'
      LOWTEMP = 'Lowest recorded temperature'
      POP80 = 'Population, 1980'
      POPSQMI = 'Population density, 1980'
      FARMPCT = '% land devoted to agriculture'
      PCTURB = '% urban pop (areas over 2,500 pop)'
      PCAPINC = '1980 per captita income'
      URB_POP = 'Urban population, 1980'
      TEMPRNGE = 'Temperature range'
      ;
RUN;

PROC PRINT DATA=STATEST N;
VAR POP80 POPSQMI PCTURB URB_POP HIGHTEMP LOWTEMP TEMPRNGE RICHFARM;
ID NAME;
TITLE 'State-Level Data for Demo Program';
RUN;

PROC MEANS MAXDEC=2 N NMISS MIN MAX MEAN;
RUN;
```

Check the SAS "listing" file for error messages. To print 2 copies off the mainframe type: "lpr < filename >(form xrev copies 2)." To copy one file to another type: "copy < filename1 > < filename2 > ." To delete a file type "erase."

A SAS data step makes raw data into a meaningful format. SAS PROCS operate on the data sets, never on raw data. Before writing a SAS data step, consider:

1. What are you going to call the SAS data set?
2. Where is the raw data located?
3. How is the data laid out?

Every SAS data step begins with the DATA statement. DATA < filename >; Next, if the data is stored in an external file, you need to tell SAS where that is. INFILE 'location'; Two options that can be used are;

- FIRSTOBS = n; * which record to start with;
- OBS = n; * which record to end with;

Example: INFILE 'HW1.SAS' FIRSTOBS=3 OBS=10;

Finally, tell SAS how the data is arranged with the INPUT statement.

1. Name the variables.
2. Tell SAS where the variables can be found.

Different forms of INPUT:

10.1.1 Reading Raw Data Assignment

```
* Demonstates reading raw data from a CMF file, and the input
  of raw data instream. The three approaches shown below create
  identical datasets and thus identical output(i.e. the same
  listing file). Create a new file containing this code, then
  run the job. Print the SAS file and the LISTING file;

* Approach 1;

DATA PRES1;
  INFILE 'MRPRES RAW A';
  INPUT NAME $ 1-20 PARTY $ 21-29 BORN 31-34 BORNST $ 37-38
        INAUG 43-46 AGEINAUG 51-52 AGEDEATH 56-57;
  IF (INAUG<1950) THEN DELETE;
RUN;

PROC PRINT DATA=PRES1;
TITLE 'Presidents elected after 1950';


* Approach 2;

FILENAME USLEADRS 'MRPRES RAW A';
DATA PRES2;
  INFILE USLEADRS;
  INPUT NAME $ 1-20 PARTY $ 21-29 BORN 31-34 BORNST $ 37-38
        INAUG 43-46 AGEINAUG 51-52 AGEDEATH 56-57;
  IF (INAUG<1950) THEN DELETE;
RUN;

PROC PRINT DATA=PRES2;
TITLE 'Presidents elected after 1950';

* Approach 3;

DATA PRES3;
  INPUT NAME $ 1-20 PARTY $ 21-29 BORN 31-34 BORNST $ 37-38
        INAUG 43-46 AGEINAUG 51-52 AGEDEATH 56-57;
  CARDS;
Eisenhower              rep     1890 tx 1953    62      78
Kennedy                 dem     1917 ma 1961    43      46
Johnson, L.             dem     1908 tx 1963    55      64
Nixon                   rep     1913 ca 1969    56      .
Ford                    rep     1913 ne 1974    61      .
Carter                  dem     1924 ga 1977    52      .
Reagan                  rep     1911 il 1981    69      .
Bush                    rep     1924 ma 1989    64      .
Clinton                 dem     .    ar 1993    .       .
;
RUN;

PROC PRINT DATA=PRES3;
TITLE 'Presidents elected after 1950';
```

10.1.2 Printing Example

```
OPTIONS NODATE LINESIZE=72;

DATA COASTAL;
INFILE 'COASTAL RAW A';
INPUT COAST $ 1-2 OCEAN $ 3-4 STATE $ 7-8 GENCST 9-14 TIDALCST 15-21;
RUN;

PROC PRINT DATA=COASTAL;
TITLE 'Take all defaults';
RUN;

PROC PRINT DATA=COASTAL SPLIT=' ' N;
VAR OCEAN STATE GENCST TIDALCST;
LABEL TIDALCST = 'Detailed outline';
SUM _NUMERIC_;
BY COAST;
FORMAT GENCST TIDALCST COMMA7.;
TITLE 'Use VAR, FORMAT, BY, And SUM statements';
TITLE2 'Use TIDALCST label for column header, print # of obs';
RUN;
```

10.1.3 Inputting Raw Data

The different ways to input data are as follow:

1. List — the variables seperated by a space. $ indicates a character variable. It can be upto 200 characters long. The $ follows the character variable name.

2. Column Input — identify exactly which columns to look-in for the variable's data.

3. Format — Example: @52 2. – the dot tells SAS this is a format. The @52 says start at column 52 to read the data. The 2. means to read two columns for numeric data. 4.0 would mean to read no decimal places. 4.2 means to read two decimal places. Ex: 1956 is read as 19.56 with the 4.2 format.

The chart on page 24 in the text book summarizes the input formats. A "comma" lets SAS know that there are commas in the raw data and should be read as numeric.

10.1.4 INPUT Formats Assignment

This assignment is not that different from the first two, except that now you will write the code yourself. The problem is to take the raw data file NATLPARK RAW, read it into a SAS job which creates a SAS dataset, and then print it out. This will require one fairly simple DATA step and one PROC. Most of this material is covered in Chapter 3 of the text book and in the example from the first class and the first homework. For a brief description of the raw data, see the bottom of this assignment.

So that you will learn these techniques, in the INPUT statement read at least one variable with column input, read at least one variable with formatted input, and use the @col specification at least once.

Also, in the DATA step, assign a descriptive label to each variable. the LABEL statement is covered on page 43 of the text book. Make sure that the labels appear when you print the dataset(use the L option in PROC PRINT).

Variables Name	Label	Type	Raw Data Cols	Format	Min	Max
PARK	Park Name	char	1-20	$20.		
ST	Principal State	char	22-23	$2.		
COAST	East/West	char	26-26	$1.		
YRESTAB	Year Established	num	27-30	4.	1872	1986
ACRES	Acres in Park	num	31-39	9.	5839	8331604

```
DATA NATIONAL;
INFILE 'NATLPARK RAW A';
INPUT PARK $ 1-20 ST $ 22-23 COAST $ 26-26 @27 YRESTAB 4. @31 ACRES 9.;
LABEL  PARK = 'PARK NAME'
       ST = 'PRINCIPAL STATE'
 COAST = 'EAST/WEST OF MISSISSIPPI RIVER'
 YRESTAB = 'YEAR ESTABLISHED'
 ACRES = 'ACRES IN PARK';

PROC PRINT DATA=NATIONAL L;
VAR PARK ST COAST YRESTAB ACRES;
TITLE 'SIZE AND HISTORY OF US NATIONAL PARKS';
RUN;
```

10.1.5 Permanent Data Sets

A SAS dataset has 2 major components:

1. The data — rectangular array where columns are the variables and rows are the observations.

2. Descriptor information — contains the number of observations, the size of the observations, date last modified, formats, labels, variable names, etc.

Temporary SAS datasets disappear when the job finishes running. Permanent SAS datasets are stored on disk and so are available for future SAS jobs without the need for a data step. Every SAS dataset has a library name in addition to the dataset name we have been using. Library names "WORK.*" are temporary. Change this with "DATA EX1HW1.STATES" which is LIBNAME.DATASETNAME. On CM, this file shows up as "STATES EX1HW1."

10.1.6 Options when Reading Datasets

Suppose you want to modify a SAS dataset that already exists. SAS dataset options can be used whenever the name of a dataset is invoked. They appear in parentheses directly following the dataset name.

- DROP — specifies variables to be dropped from the dataset(DROP = <var1> <var2> ...).
- KEEP — specifies variables to be kept in the dataset(KEEP = <var1> <var2> ...).
- RENAME — change the variable name in the dataset(RENAME = (OLDNAME = NEWNAME)).
- LABEL — gives a label to a dataset(LABEL = 'US PRESIDENTS').
- OBS and FIRSTOBS — (FIRSTOBS = n) specifies the first observation to be read. (OBS = n) specifies the last observation to read.
- WHERE — specifies a condition for an observation to be read into a dataset(WHERE = (conditions)).

10.1.7 Creating SAS Variables Assignment

```
OPTIONS LS = 132;
DATA VALID;

INFILE 'VALID DAT A';
INPUT ID 1-6 SATFATDR 8-15 SATFATFF 17-24 TOTFATDR 26-33
      TOTFATFF 35-42 ALCONDR 44-51 ALCONFFQ 53-60
      TOTCALDR 62-70 TOTCALFF 72-80;

DIFDRFFQ = SATFATDR - SATFATFF;
DIFTOT = TOTFATDR - TOTFATFF;
DIFFALCON = ALCONDR - ALCONFFQ;
DIFCAL = TOTCALDR - TOTCALFF;

* SUBJECT CONFORMS;

IF ((SATFATDR>=SATFATFF)AND(ALCONDR>=ALCONFFQ)AND(TOTFATDR>=TOTFATFF)
    AND(TOTCALDR>=TOTCALFF)) OR
   ((SATFATDR<=SATFATFF)AND(ALCONDR<=ALCONFFQ)AND(TOTFATDR<=TOTFATFF)
    AND(TOTCALDR<=TOTCALFF))
    THEN CONFORM = "CONFORM   ";

* WHICH SUBJECT CONFORMS?;

IF ((SATFATDR>=SATFATFF)AND(ALCONDR>=ALCONFFQ)AND(TOTFATDR>=TOTFATFF)
    AND(TOTCALDR>=TOTCALFF))
    THEN IDNT = "DR   ";

IF ((SATFATDR<=SATFATFF)AND(ALCONDR<=ALCONFFQ)AND(TOTFATDR<=TOTFATFF)
    AND(TOTCALDR<=TOTCALFF))
    THEN IDNT = "FFQ  ";

...etc...
```

10.2 PROC CONTENTS Assignment

PROC CONTENTS is used to display the descriptor information associated with every SAS dataset.

```
OPTIONS LS = 132;
DATA HW5.RATIOS;
SET HW5.VALID;

RATDRFFQ = SATFATFF/SATFATDR;
RATTOT = TOTFATFF/TOTFATDR;
RATALCON = ALCONFFQ/ALCONDR;
RATCAL = TOTCALFF/TOTCALDR;

LABEL RATDRFFQ = 'RATIO OF DR:FFQ FOR FAT'
      RATTOT = 'RATIO OF TOTAL FAT'
RATALCON = 'RATIO OF DR:FFQ FOR ALCOHOL'
RATCAL = 'RATIO OF TOTAL ALCOHOL';

PROC CONTENTS DATA = HW5.RATIOS;
```

```
RUN;
```

10.3 PROC MEANS

Here is a SAS example using PROC MEANS:

```
OPTIONS LS = 72;

DATA STATES;
INFILE 'STATES1 RAW A';
INPUT NAME $ 4-19 HIGHTEMP 25-27 LOWTEMP 29-31
      POP80 POPSQMI FARMPCT PCTURB @83 PCAPINC 5.;

URB_POP = (PCTURB*POP80)/100;
TEMPRNGE = HIGHTEMP - LOWTEMP;
IF ((FARMPCT>50)&(PCAPINC>7000)) THEN RICHFARM = 'YES';
ELSE RICHFARM = 'NO';

FORMAT POP80 URB_POP COMMALL. FARMPCT PCTURB 6.2 PCAPINC DOLLAR8.;
LABEL NAME = 'STATE NAME'
      HIGHTEMP = 'HIGEST RECORDED TEMPERATURE'
LOWTEMP = 'LOWEST RECORDED TEMPERATURE'
POP80 = 'POPULATION, 1980'
POPSQMI = 'POPULATION DENSITY, 1980'
FARMPCT = '% LAND DEVOTED TO AGRICULTURE'
PCTURB = '% URBAN POP(AREAS OVER 2,500 POP)'
PCAPINC = '1980 PER CAPITA INCOME'
URB_POP = 'URBAN POPULATION, 1980'
TEMPRNGE = 'TEMPERATURE RANGE';
RUN;

PROC MEANS DATA=STATES MAXDEC=1;
VAR HIGHTEMP LOWTEMP TEMPRNGE POP80;
RUN;

PROC SORT DATA=STATES;
BY RICHFARM;
RUN;

PROC MEANS DATA=STATES MAXDEC=1 N MEAN RANGE STD;
CLASS RICHFARM;
VAR HIGHTEMP LOWTEMP TEMPRNGE POP80;
RUN;
```

10.3.1 PROC MEANS Assignment

We will use the permanent dataset with 19 variables that you created in the previous assignment to try out some of the PROCs we have learned.

1. It has been discovered that observations #34 and #140 were erroneously recorded. So you need to delete them from your dataset. DO this first, creating a new permanent dataset with only 171 observations, but with all 19 variables. This will be the dataset that we work with from now on. You should be able to do this with a SET statement. Do NOT start from the beginning with the raw data!

2. Print the data so that it is grouped into the three categories CONFORM, SPLIT, and NONCONF that are given by the values of the first character variable that you created in assignment 4. Use subject's id number as an ID variable. Have the PRINT also show labels, and have it tell you how many measurements are in each of the three groups. Also, show the overall sum for each of four difference variables you created in assignment 4. What do these sums suggest?

   The difference between alcohol consumption DR and alcohol consumption FFQ is neglible. The difference between total fat seems to favor the DR variable some what. The differences of total calories seems to favor the DR variable significantly. The DR-FFQ difference sum is positive indicating favoring DR.

3. Now use the MEANS procedure to get the same information obtained with PRINT above, and obtain means as well as sums. However, not get the values only for the four difference variables. Also, run a t-test for significance of the four difference variables, including p-values for the t-tests(the t-tests are for all of the data, not the grouped data). All of this can be done with two seperate PROC MEANS. What do you conclude from the t-tests?

   The DR-FFQ differences, differences of total fat and differences of total calories are highly significant. The alcohol differences is negligible.

```
OPTIONS LS = 130;
DATA HW5.MISSING;
SET HW5.RATIOS;

IF (_N_ = 34)OR(_N_ = 140) THEN DELETE;

PROC SORT;
BY CONFORM;

PROC PRINT DATA = HW5.MISSING L N;
VAR SATFATDR SATFATFF TOTFATDR TOTFATFF ALCONDR ALCONFFQ
    TOTCALDR TOTCALFF DIFDRFFQ DIFTOT DIFALCON DIFCAL IDNT;
ID ID;
BY CONFORM;
SUM DIFDRFFQ DIFTOT DIFALCON DIFCAL;
TITLE 'FOOD FREQUENCY QUESTIONAIRE';
RUN;

PROC MEANS DATA=HW5.MISSING N MEAN SUM;
BY CONFORM;
ID ID;
VAR DIFDRFFQ DIFTOT DIFALCON DIFCAL;
TITLE 'FOOD FREQUENCY GROUPED BY CONFORMITY';
RUN;

PROC MEANS DATA=HW5.MISSING T PRT MEAN SUM;
VAR DIFDRFFQ DIFTOT DIFALCON DIFCAL;
TITLE 'FOOD FREQUENCY STUDENT T TESTS OF DIFFERENCES';
RUN;
```

10.4 PROC UNIVARIATE

The options for PROC UNIVARIATE are:

- DATA = <dataset> .
- FREQ — produces a frequency table for the data.
- NORMAL — test for normality of the data.
- PLOT — stem/leaf plot, boxplot, and Q-Q plot.
- NOPRINT — makes the procedure run, but does not print anything.

Here are 3 examples using PROC UNIVARIATE:

```
* A MANUFACTURER OF MICROWAVE OVENS TESTS PERIODICALLY
  FOR THE AMOUNT OF RADIATION THEY OMIT. A SAMPLE OF 42
  OVENS IS OBTAINED, AND THE EMISSIONS(WITH DOOR CLOSED)
  MEASURED FOR EACH. CAN IT BE CONCLUDED THAT THE AVERAGE
  EMMISSION FALLS BELOW THE STANDARD OF .15 UNITS?;

OPTIONS NODATE LINESIZE=72 PAGESIZE=40;

DATA MICRO;
INFILE 'MWOVEN DAT A';
INPUT EMIT;
EXCESS=EMIT-.15;
LABEL EMIT = 'RADIATION EMITTED WITH DOOR CLOSED'
      EXCESS = 'UNITS OF RADIATION OVER .15';

PROC UNIVARIATE DATA=MICRO FREQ PLOT NORMAL;
VAR EXCESS;
TITLE 'LEFTOVERS AGAIN?';
RUN;

*THE DATA USED HERE IS FROM A STUDY OF ANESTHETICS PERFORMED
 ON DOGS. EACH DOG WAS GIVEN THE DRUG PENTOBARBITOL. TWO
 MEASUREMENTS WERE THEN TAKEN, ONE WITH HALOTHANE
 ADMINISTERED, AND ONE WITHOUT. THE MEASURES ARE
 MILLISECONDS BETWEEN HEARTBEATS. DOES USE OF HALOTHANE
 MAKE FOR A MORE EFFECTIVE ANESTHETIC?;

OPTIONS NODATE LINESIZE=72 PAGESIZE=40;

DATA DOGS;
INFILE 'DOG DAT A';
INPUT X1 X2;
DIFF = X1-X2;
LABEL X1 = 'RESPONSE WITHOUT HALOTHANE'
      X2 = 'RESPONSE WITH HALOTHANE'
DIFF = 'DIFFERENCE OF RESPONSES';

PROC UNIVARIATE DATA=DOGS FREQ PLOT NORMAL;
VAR DIFF;
TITLE 'LET SLEEPING DOGS LIE';
RUN;

 DATA STATES;
 INFILE 'STATES1 RAW A';
 INPUT NAME $ 4-19 HIGHTEMP 25-27 LOWTEMP 29-31
```

```
        POP80 POPSQMI FARMPCT PCTURB
        @83 PCAPINC 5.;
 URB_POP = (PCTURB * POP80) / 100;
 TEMPRNGE = HIGHTEMP - LOWTEMP;
 IF  ((FARMPCT>50)&(PCAPINC>7000)) THEN RICHFARM = 'YES';
 ELSE RICHFARM = 'NO';

 FORMAT POP80 URB_POP COMMA11. FARMPCT PCTURB 6.2 PCAPINC DOLLAR8.;
 LABEL NAME = 'State name"
       HIGHTEMP = 'Highest recorded temperature'
       LOWTEMP = 'Lowest recorded temperature'
       POP80 = 'Population, 1980'
       POPSQMI = 'Population density, 1980'
       FARMPCT = '% land devoted to agriculture'
       PCTURB = '% urban pop (areas over 2,500 pop)'
       PCAPINC = '1980 per captita income'
       URB_POP = 'Urban population, 1980'
       TEMPRNGE = 'Temperature range'
       ;
 RUN;


PROC SORT DATA=STATES;
BY RICHFARM;

PROC UNIVARIATE DATA=STATES FREQ PLOT NORMAL;
VAR POP80;
BY RICHFARM;
ID NAME;
RUN;
```

10.4.1 PROC UNIVARIATE Assignment

This week we analyze aspects of our favorite dataset using PROC UNIVARIATE. Use the permanent dataset with 19 variables and 171 observations that you created in the previous assignment.

1. For each of the four difference variables created, use UNIVARIATE to examine the shapes of their distributions. Do any of them appear to be skewed? Do they appear to be reasonably normal? What is the result of the test for normality? Also, what do the sign test, the sign rank test, and the t-test tell you? Do you prefer the nonparametric tests over the t-test for any of the four variables? Why or why not?

   When the data is not normally distributed, use the non-parametric tests. When the data is normally distributed, use the t-tests. The hypotheses are $H_0 : \mu = 0$ vs $H_1 : \mu \neq 0$. Reject H_0 for small p-values.

2. Repeat what you have done for (1), answering the same questions, but use the ratio variables created in the previous assignment. This will let you compare the two methods from a different perspective. However, first subtract 1 from every ratio variable. What is the purpose of this?

   We subtracted 1 from each ratio variable so the test $\mu = 0$ will match with what SAS tests for.

```
OPTIONS LINESIZE = 72;

DATA RATIOS.MINUS1;
```

```
SET HW5.MISSING;

RAT1 = RATDRFFQ - 1;
RAT2 = RATTOT - 1;
RAT3 = RATALCON - 1;
RAT4 = RATCAL - 1;

LABEL RAT1 = 'RATIO OF DR/FFQ MINUS 1'
RAT2 = 'RATIO OF TOTAL FAT MINUS 1'
RAT3 = 'RATIO OF ALCOHOL MINUS 1'
RAT4 = 'RATIO OF CALORIES MINUS 1';

PROC UNIVARIATE DATA=HW5.MISSING NORMAL PLOT;
VAR DIFDRFFQ DIFTOT DIFALCON DIFCAL;
ID ID;
TITLE 'ANALYSIS OF DIFFERENCES';
RUN;

PROC UNIVARIATE DATA=RATIOS.MINUS1 NORMAL PLOT;
VAR RAT1 RAT2 RAT3 RAT4;
ID ID;
TITLE 'ANALYSIS OF RATIOS';
RUN;
```

10.5 PROC FREQ and PROC CHART

The following code will make a 2D table of frequencies:

```
PROC FREQ;
TABLES HEIGHT*GRADE;
```

The syntax of PROC CHART is:

```
PROC CHART;
VBAR <FIELD1> /GROUP = <FIELD2> TYPE = PERCENT G100;
```

Here is an example using PROC FREQ and PROC CHART:

```
PROC FREQ DATA=PRES.US ORDER = FREQ;
TABLES PARTY REGION/NOCUM;
TABLES BORNST;
RUN;

PROC CHART DATA=PRES.US(WHERE(INAUG>1866));
HBAR PARTY;
VBAR PARTY/GROUP=REGION TYPE=PERCENT;
VBAR PARTH/TYPE=MEAN SUMVAR=AGEDEATH;
VBAR AGEINQUG/MIDPOINTS=45 TO 70 BY 5 NOSPACE;
RUN;
```

10.5.1 PROC FREQ/PROC CHART Assignment

This week we analyze aspects of the FFQ/DR dataset using PROC FREQ and PROC CHART. Use the permanent dataset with 19 variables and 171 observations.

1. Make a frequency table that shows how many individuals are in each of the CONFORM, NONCONF, and SPLIT categories.

2. Make a chart that shows the same information in (1).
3. Make a chart that shows for each of the CONFORM and NONCONF categories, how many individuals have more of the 4 measurements higher using the FFQ method, and how many have more than the 4 higher using the DR method. To make this chart you need only use the two character variables.
4. Based on the charts above, does it appear that, overall for the four variables(saturated fat, total fat, alcohol, and total calories) being measured, the FFQ and DR methods are comparable? Explain.
5. Thinking back to the results from the previous two assignments, do you think the FFQ method is a suitable substitute for the DR method for any of the four variables? Explain.

```
PROC FREQ DATA=HW5.MISSING ORDER = FREQ;
TABLES CONFORM;
TITLE 'FREQUENCY TABLE OF FOOD QUESTIONNAIRE';
RUN;

PROC CHART DATA=HW5.MISSING;
HBAR CONFORM;
TITLE 'BAR CHART OF FOOD QUESTIONNAIRE';
RUN;


PROC CHART DATA=HW5.MISSING(WHERE=((CONFORM='CONFORM')OR
                                    CONFORM='NONCONFORM')));
VBAR CONFORM/GROUP = IDNT;
TITLE 'BAR CHART OF FOOD QUESTIONNAIRE BY DR AND FFQ';
RUN;
```

10.6 Combining Datasets and Handling Dates

1. Stacking — adding to the bottom of a dataset. Also called concatenation. Purpose: to create a dataset that contains all measurements from dataset 1, followed by all measurements from dataset2, and so on. Syntax: DATA —–; SET DATASET1(OPTIONS) DATASET2(OPTIONS) ....
2. Interleaving — similar to concatenation except that observations from one dataset are not all above or below those of another dataset. Instead, they are put in the new dataset in an order specified by a certain variable which we shall refer to as the "by" variable. Syntax: DATA —–; SET DATASET1 DATASET2 ...; BY VARNAME; The "by" variable must be in both datasets.
3. Matched Merge — find matching id's and add data to that line(2nd dataset overwrites the first data set). Syntax: DATA —–; MERGE DATASET1 DATASET2 ...; BY VARNAME; If there are no matching variable names in the 2 datasets, then a new column is created.

SAS provides an easy way of addressing the question: how long something took given 2 dates. When reading the data, do 1) read date values with a special date input format, 2) SAS stores the date as a number which is the number of days before or after January 1, 1960.

10.6.1 Assignment

1. The raw data files that you need for this assignment are named HW9DAT ONE and HW9DAT TWO. They are located on the account F3525605@ODUVM.CC.ODU.EDU. Use ftp to retrieve theses files. The password for this account is ORIORLE.
2. The first file contains measurements on three variables: subject's id number, subject's date of birth, and date on which the subject entered the study. The second file contains measurements on two

variables: subject's id and date of first followup on the subject. Create a SAS dataset out of each of these raw data files. Be sure to use the correct in format to read the dates.

3. Merge the two datasets so that you have one SAS dataset with four variables for each subject. Now calculate the following three variables: 1) age, to the nearest .1 years, at which the subject entered the study, 2) the number of weeks, to the nearest week, between entry and first followup, and 3) the age-group to which the subject belonged at time of entry into the study. To do the last, use these three age groups: <= 29.9 years, 30.0 - 40.9 years, >= 50.0 years. Print this dataset.

4. Use a frequency table to display how many subjects are in each age group.

```
DATA MEASURE1.DAT;
INFILE 'HW9DAT ONE A';
INPUT @1 ID 5. @7 BIRTH MMDDY8. @16 ENTRY MMDDYY8.;
LABEL ID = 'IDENTIFICATION'
BIRTH = 'DATE BORN'
ENTRY = 'DATE ENTERED STUDY';

PROC SORT; BY ID;

DATA MEASURE2.DAT;
INFILE 'HW9DAT TWO A';
INPUT @1 ID 5. @7 FOLLOW MMDDYY8.;

PROC SORT; BY ID;

LABEL FOLLOW = 'DATE OF FIRST FOLLOW-UP'
ID = 'IDENTIFICATION';

DATA MERGED.BOTH;
MERGE MEASURE1.DAT MEASURE2.DAT;
BY ID;


ENTRYAGE = (ENTRY-BIRTH)/365.25;
WEEKS = (FOLLOW-ENTRY)/7;
IF ENTRYAGE<=29.9 THEN CAT = 'UNDER 29.9 YEARS OLD';
ELSE
IF ENTRYAGE>=50 THEN CAT = 'OVER 50 YEARS OLD;
ELSE CAT = 'BETWEEN 30 AND 49.9 YEARS OLD';

LABEL ENTRYAGE = 'AGE OF ENTRY'
WEEKS = '# WEEKS BETWEEN ENTRY AND FOLLOW-UP'
CAT = 'AGE GROUP';

PROC PRINT L;
ID ID;
FORMAT BIRTH MMDDYY8. ENTRY MMDDYY8. FOLLOW MMDDYY8.
       ENTRYAGE 5.1 WEEKS 5.1;
VAR BIRTH ENTRY FOLLOW ENTRYAGE WEEKS CAT;
TITLE 'STUDY GROUP';
RUN;

PROC FREQ ORDER=FREQ;
TABLES CAT;
```

```
TITLE 'FREQUENCY TABLE BY AGE GROUP';
RUN;
```

10.7 PROC FORMAT

PROC FORMAT controls the formatting of printing on paper. PROC FORMATS are user defined. The syntax is

```
PROC FORMAT;
VALUE FMTNAME
RANGE1 = 'TEXT'
RANGE2 = 'TEXT'
...
RANGEN = 'TEXT';
```

FMTNAME is the name of you format. It can be 1–8 characters. It cannot begin with #. If the name is a format for a character variable, it must begin with $.

10.7.1 PROC FORMAT Assignment

In this assignment you will make a new SAS dataset, create formats for some of the variables, and use those formats in examining relationships among a few variables.

1. The raw data file is HSB DAT, which will be sent to your account. The data is described on the accompanying sheet.
2. Create a SAS dataset containing the 15 variables. Use the same names as shown on the handout.
3. Make formats for the following variables, so that their numeric values are replaced by the character strings shown on the handout: SES, SCTYP, HSP.
4. Using your formats, make the following two-way tables: SES vs SCTYP and SES vs HSP. In each table, make SES the row variable, and show percentages in the rows only.
5. Do you see an apparent relationship between SES and SCTYP? What is the nature of that relationship? Explain.
6. Do you see an apparent between SES and HSP? What is the nature of that relationship? Explain.

```
DATA SCHOOL;
INFILE 'HSB DAT A';
INPUT ID SEX RACE SES SCTYP HSP LOCUS CONCPT MOT CAR
RDG WRTG MATH SCI CIV;

PROC FORMAT;
VALUE SESFORM
1 = 'LOWER'
2 = 'MIDDLE'
3 = 'UPPER';

VALUE SCHFORM
1 = 'PUBLIC'
2 = 'PRIVATE';

VALUE HSPFORM
1 = 'GENERAL'
2 = 'ACADEMIC'
```

```
3 = 'VOCATIONAL';
RUN;

PROC FREQ;
TABLES SES*SCTYP SES*HSP/ NOCOL NOPERCENT;
FORMAT SCTYP SCHFORM. HSP HSPFORM. SES SESFORM.;
TITLE 'SOCIO-ECONOMIC STATUS VS SCHOOL TYPE AND HS PROGRAM';
RUN;
```

10.8 Data Analysis PROCS

PROC TTEST can be used to perform a t-test on a mean response. The null hypothesis is that $\mu = 0$.

```
PROC TTEST DATA = <DATASET NAME.;
CLASS <FIELDNAMES1>;
VAR <FIELDNAMES2>;
RUN;
```

PROC CORR performs an Spearman correlation analysis. The hypotheses are H_0 : correlation is zero, H_1 : correlation is not zero. PROC CORR is used to look at the relationship between two variables. PROC REG is used to perform a regression analysis. Type I sums of squares tells the significance of a variable given the previous ones are already in the model.

10.8.1 Assignment

```
DATA SCHOOL;
INFILE 'HSB DAT A';
INPUT ID SEX RACE SES SCTYP HSP LOCUS CONCPT
MOT CAR RDG WRTG MATH SCI CIV;

LABEL ID = 'ID NUMBER'
SEX = 'SEX'
RACE = 'RACE'
SES = 'SOCIO-ECONOMIC STATUS'
SCTYP = 'SCHOOL TYPE'
HSP = 'HIGH SCHOOL PROGRAM'
LOCUS = 'LOCUS OF CONTROL'
CONCPT = 'SELF CONCEPT'
MOT = 'MOTIVATION'
CAR = 'CAREER CHOICE'
RDG = 'READING T-SCORE'
WRTG = 'WRITING T-SCORE'
MATH = 'MATH T-SCORE'
SCI = 'SCIENCE T-SCORE'
CIV = 'CIVICS T-SCORE';

PROC FORMAT;
VALUE SESFORM
1 = 'LOWER'
2 = 'MIDDLE'
3 = 'UPPER';

VALUE SCHFORM
1 = 'PUBLIC'
```

```
2 = 'PRIVATE';

VALUE HSPFORM
1 = 'GENERAL'
2 = 'ACADEMIC'
3 = 'VOCATIONAL';

VALUE MATHFORM
LOW-25 = 'LOWER 25%'
25.0001-50 = '25%-50%'
50.0001-75 = '50%-75%'
75.0001-HIGH = 'TOP 25%';
RUN;

PROC CHART;
VBAR MATH/GROUP=SCTYP TYPE=PERCENT G100;
FORMAT SCTYP SCHFORM.;
TITLE 'BAR CHART OF SCHOOL TYPE VS MATH SCORES';
RUN;

PROC TTEST;
CLASS SCTYP;
VAR MATH;
TITLE 'T-TESTS OF SCHOOL TYPE AND MATH SCORES';
RUN;

PROC SORT; BY SCTYP;

PROC UNIVARIATE PLOT;
BY SCTYP;
VAR MATH;
FORMAT SCTYP SCHFORM.;
TITLE 'PLOT OF SCHOOL TYPE AND MATH SCORES';
RUN;

PROC CHART;
VBAR MATH/GROUP=SES SUBGROUP=SCTYP TYPE=PERCENT G100;
FORMAT SES SESFORM. SCTYP SCHFORM.;
TITLE 'BAR CHART OF SOCIO-ECONOMIC STATUS/SCHOOL
 TYPE AND MATH SCORES';
RUN;

PROC GLM;
CLASS SCTYP SES;
MODEL MATH = SCTYP SES SCTYP*SES;
MEANS SCTYP SES SCTYP*SES;
TITLE 'MODEL OF MATH SCORES AS A FUNCTION OF SOCIO-
 ECONOMIC STATUS AND SCHOOL TYPE';
RUN;
```

Chapter 11

Linear Regression

Dr. Morgan, Old Dominion University
Statistics 537, Fall 1996
Text used: Linear Statistical Models, an Applied Approach, 2nd edition, Bruce L. Bowerman and Richard T. O'Connell, Duxbury Press, 1990.

11.1 Simple Linear Regression

The simplest form of the technique known as regression is that of predicting a single variable y from a single variable x using a straight line relationship. Consider this imaginary example: y is a child's weight and x is the average of the parent's heights. We obtain n measurements on x and y. Call them (x_1, y_1), $(x_2, y_2), \ldots$ (x_n, y_n). We postulate a *linear model* relating the mean of y_i to x_i. $y_i = \mu_i + \epsilon_i = \beta_0 + \beta_1 x_i + \epsilon_i$, where μ_i is the mean of y_i for all children whose parents' average height is x_i. ϵ_i is a random variable representing random variance of y_i from μ_i. $\mu_i = \beta_0 + \beta_1 x_i$ is the linear model for μ_i. β_0 is the intercept and β_1 is the slope.

Important Note: We do not know if this model is true, and in a real sense, no model is ever true. Models are mathematical approximations of reality, and we hope to find one that does a good job of approximation. We are now entertaining a simple linear model, which we will "fit(estimate)." Later, we will learn how to measure the adequacy of the model. First, we learn how to fit the model. We will use the data $(x_1, y_1), \ldots$ to find estimates b_0 of β_0 and b_1 of β_1. They in turn will give $\widehat{y} = b_0 + b_1 x$. $\widehat{y}$ is the predicted value of y for a given x. To find b_0 and b_1 we us the technique of *least squares.* Here is the idea: out model is $y_i = \beta_0 + \beta_1 x_i + \epsilon_i$. We choose the values b_0 and b_1 that makes the deviations "small." Specifically, we will minimize the sum of squared deviations.

$$s = \sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2.$$

β_0 moves the line up and down. β_1 changes the tilt of the line.

$$\frac{\partial s}{\partial \beta_0} = -2 \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i), \quad \frac{\partial s}{\partial \beta_1} = -2 \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i) x_i.$$

Set these two equations equal to zero and solve for β_0 and β_1.

$$\left.\begin{array}{l} \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i) = 0 \\ \sum_{i=1}^{n} x_i (y_i - \beta_0 - \beta_1 x_i) = 0 \end{array}\right\}$$

$$\left.\begin{array}{l} \sum_{i=1}^{n} y_i - n b_0 - b_1 \sum_{i=1}^{n} x_i = 0 \\ \sum_{i=1}^{n} x_i y_i - b_0 \sum_{i=1}^{n} x_i - b_1 \sum_{i=1}^{n} x_i^2 = 0 \end{array}\right\}$$

Then,

$$\left.\begin{array}{l} b_0 n + b_1 \sum_{i=1}^n x_i = \sum_{i=1}^n y_i \\ b_0 \sum_{i=1}^n x_i + b_1 \sum_{i=1}^n x_i^2 = \sum_{i=1}^n x_i y_i \end{array}\right\}$$

The above two equations are called *normal equations.* The solution is:

$$b_1 = \frac{n \sum_{i=1}^n x_i y_i - \left(\sum_{i=1}^n x_i\right)\left(\sum_{i=1}^n y_i\right)}{n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i\right)^2} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2},$$

where $\bar{x}$ is the average of the x's and $\bar{y}$ is the average of the y's. $\bar{x} = \frac{1}{n}\sum_{i=1}^n x_i$, and $\bar{y} = \frac{1}{n}\sum_{i=1}^n y_i$.

$b_0 = \bar{y} - b_1\bar{x}$. Substituting back into the model equation gives:

$$\widehat{y} = b_0 + b_1 x = \bar{y} - b_1\bar{x} + b_1 x = \bar{y} + b_1(x - \bar{x}).$$

We now have a line. We next need to find methods for judging how well this line "fits the data." Consider the identity

$$y_i - \bar{y} = (y_i - \widehat{y}_i) + (\widehat{y}_i - \bar{y}).$$

Square both sides:

$$(y_i - \bar{y})^2 = (y_i - \widehat{y}_i)^2 + (\widehat{y}_i - \bar{y})^2 + 2(y_i - \widehat{y})(\widehat{y}_i - \bar{y}).$$

Sum both sides:

$$\sum_{i=1}^n (y_i - \bar{y})^2 = \sum_{i=1}^n (y_i - \widehat{y}_i)^2 + (\widehat{y}_i - \bar{y})^2 + 2(y_i - \widehat{y}_i)(\widehat{y}_i - \bar{y}).$$

Working with the cross product terms only:

$$2\sum_{i=1}^n (y_i - \widehat{y}_i)(\widehat{y}_i - \bar{y}) = 2\sum_{i=1}^n (y_i - \widehat{y}_i)(b_1(x_i - \bar{x})) = 2b_1(y_i - \widehat{y}_i)(x_i - \bar{x}) =$$

$$2b_1 \sum_{i=1}^n [y_i - \bar{y} - b_1(x_i - \bar{x})](x_i - \bar{x}) = 2b_1\left[\sum_{i=1}^n (y_1 - \bar{y})(x_i - \bar{x}) - b_1 \sum_{i=1}^n (x_i - \bar{x})^2\right] =$$

$$2b_1 \sum_{i=1}^n (y_i - \bar{y})(x_i - \bar{x}) - \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}) = 0.$$

Hence,

$$\sum_{i=1}^n (y_i - \bar{y})^2 = \sum_{i=1}^n (y_i - \widehat{y}_i)^2 + \sum_{i=1}^n (\widehat{y}_i - \bar{y})^2.$$

Page 117 in the textbook shows b_1 and b_0 derived.

$$SS(TOTAL) = \sum_{i=1}^n (y_i - \bar{y})^2, \quad SS(ERROR) = \sum_{i=1}^n (y_i - \widehat{y}_i)^2.$$

We want $SS(ERROR)$ to be small. $SS(REGRESSION) = \sum_{i=1}^n (\widehat{y}_i - \bar{y})^2$. We want $SS(REGRESSION)$ to be large. The proportion of total variation explained by the model is $R^2 = \frac{SS(REGRESSION)}{SS(TOTAL)} = 1 - \frac{SS(ERROR)}{SS(TOTAL)}$. This quantity R^2 is used in any regression model, not just the simple linear regression.

This statistic leads to a simple technique to verify the integrity of the data loaded into a database. Model the database data as the dependent variable y and the actual source data x using linear regression. If the data loaded correctly, then the x variable should exactly predict the y variable, $R^2 = \%100$.

$$R^2 = \frac{SS(Regression)}{SS(TOTAL)} = \frac{\sum_{i=1}^{\infty}(\widehat{y}_i - \bar{y})^2}{\sum_{i=1}^{\infty}(y_i - \bar{y})^2} = \frac{\sum_{i=1}^{n}[\bar{y} - b_1(x_i - \bar{x}) - \bar{y}]^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} =$$

$$\frac{b_1^2 \sum_{i=1}^{n}(x_i - \bar{x})^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} = \frac{\left[\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})\right]^2 \sum_{i=1}^{n}(x_i - \bar{x})^2}{\left[\sum_{i=1}^{n}(x_i - \bar{x})^2\right]^2 \sum_{i=1}^{n}(y_i - \bar{y})^2} = \left[\frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum(x_i - \bar{x})^2}\sqrt{\sum(y_i - \bar{y})^2}}\right]^2 = r^2,$$

where r is Pierson's correlation coefficient which is a simple coefficient of determination(see Section 5.3 of the text book).

SAS Code

```
DATA REPAIR;
INPUT N_UNITS MINUTES;
CARDS;
1 23
2 29
3 49
4 64
4 74
5 87
6 96
6 97
7 109
8 119
9 149
9 145
10 154
10 166;

PROC PLOT;
PLOT MINUTES*N_UNITS;
RUN;

PROC REG;
MODEL MINUTES = N_UNITS/P;
OUTPUT OUT=NEW P=PRED R=RESID;
RUN;

PROC PLOT;
PLOT MINUTES*N_UNITS='O' PRED*N_UNITS='*'/OVERLAY;
PLOT RESID*N_UNITS='*'/VREF=0;
RUN;
```

11.1.1 Point Estimates

The model is $y_i = \mu_i + \epsilon_i = \beta_0 + \beta_1 x_i + \epsilon_i$. The *mean response* μ_0 when $x = x_0$ is $\beta_0 + \beta_1 x_0$. An estimate of the mean response when $x = x_0$ is $\widehat{y}_0 = b_0 + b_1 x_0$. A *particular response* when $x = x_0$ is $\beta_0 + \beta_1 x_0 + \epsilon_0$. So, our prediction of the response of a new measurement at $x = x_0$ is $\widehat{y}_0 = b_0 + b_1 x_0$. This matches the main response estimate because the best estimate of ϵ_0 is zero. However, this estimate is subject to more variability than that of the mean response.

11.1.2 Homework and Answers

1. The chairman of the Accounting Department at a large university undertakes a study to relate starting salary(y) after graduation for accounting majors to grade point average(GPA) in major courses. To do this, records of seven recent accounting graduates are randomly selected.

Accounting Graduate i	GPA x_i	Starting Salary, y_i (thousands of dollars)
1	3.26	28.2
2	2.60	24.8
3	3.35	27.9
4	2.86	25.3
5	3.82	30.3
6	2.21	23.0
7	3.47	29.4

(a) Plot y versus x. Explain why the plot suggests that the simple linear regression model having a positive slope $y_i = \mu_i + \epsilon_i = \beta_0 + \beta_1 x_i + \epsilon_i$ might appropriately relate y to x.

The plot of x versus y appears on the next page. Looking at the data points, the points do appear to fall on an approximate straight line. As the GPA increases, so does the starting salary of accounting graduates. Perhaps employers think that employees with a higher GPA are more productive. Thus, employee's with a higher GPA are compensated more than employee's with a lower GPA. This explains the positive slope. An increase in GPA means an increase in starting salary.

(b) Discuss the meaning of the third historical population of potential starting salaries.

(c) Discuss the meaning of μ_3, the third mean starting salary. μ_3 is the mean of the population defined in part (b).

(d) Discuss the conceptual difference between μ_3 and $y_3 = \mu_3 + \epsilon_3$. What does ϵ_3 measure in this situation?

y_3 is one observation of one individual with GPA 3.35. ϵ_3 measures how far this person's salary fell from μ_3.

(e) Discuss the meaning of β_0 and β_1 in this model. Why does the interpretation of β_0 fail to make practical sense?

Again, β_0 is the Y-axis intercept. In this study, β_0 shows the starting salary of the person with a GPA of 0.00. β_0 fails to make practical sense. No data was gathered of people who did not go to college. These people's GPA would be zero. Yet, this is not reflected in this study. β_1 represents the rise in starting salary per unit rise in GPA.

(f) Calculate the least squares point estimates b_0 and b_1 of β_0 and β_1.

$$b_1 = \frac{7\sum_{i=1}^{7} x_i y_i - \left(\sum_{i=1}^{7} x_i\right)\left(\sum_{i=1}^{7} y_i\right)}{7\sum_{i=1}^{7} x_i^2 - \left(\sum_{i=1}^{7} x_i\right)^2} = \frac{7(590.829) - (21.57)(188.9)}{7(68.3071) - (21.57)^2} = 4.752111.$$

$$b_0 = \bar{y} - b_1\bar{x} = 26.98571 - (4.752111)(3.081429) = 12.3424.$$

(g) Using the prediction equation $\hat{y}_i = b_0 + b_1 x_i$, calculate a point estimate of μ_3 and a point prediction of $y_3 = \mu_3 + \epsilon_3$.

$$\mu_3 = \beta_0 + \beta_1 x_3 = 12.34242 + (4.752111)(3.35) = 28.262.$$

$$y_3 = \mu_3 + \epsilon_3 = 28.262 + 0.0 = 28.262.$$

(h) Suppose that an accounting major will graduate with a GPA of $x_0 = 3.26$. The starting salary of this graduate may be expressed in the form $y_0 = \mu_0 + \epsilon_0$.

i. Discuss the conceptual difference between μ_0 and $y_0 = \mu_0 + \epsilon_0$.

μ_0 is the mean starting salary of all accounting majors when the GPA $x_0 = 3.26$. y_0 is the future starting salary of a future graduate. There is not an actual data point that corresponds to such a GPA for the starting salary.

ii. Is the grade point average $x_0 = 3.25$ in the experimental region?

The experimental region ranges from 2.21 to 3.82. 3.25 is in the experimental region.

iii. Using an appropriate prediction equation, calculate a point estimate of μ_0 and a point prediction of y_0.

$$\mu_0 = \beta_0 + \beta_1(3.25).$$

$$\hat{y}_0 = b_0 + b_1 x_0 = 12.34242 + (4.752111)(3.25) = 27.87.$$

(i) Calculate SSE, s^2, and s.

$$SSE = \sum_{i=1}^{7} \epsilon_i^2 = 1.061178. \Rightarrow s^2 = \frac{SSE}{n-2} = \frac{1.061178}{5} = 0.21224 \Rightarrow s = \sqrt{s^2} = 0.461.$$

2. The no-intercept model for the simple linear regression line is $Y_i = \beta X_i + \epsilon_i, i = 1, 2, 3, ..., n$. This is sometimes appropriate when the line *must* pass through the origin $(0, 0)$. For this model,

(a) Find the least squares estimate of β. (That is, find the value b for β that minimizes the sum of squared errors for this model).

$$s^2 = \sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} (Y_i - \beta X_i)^2 . \frac{\partial s}{\partial \beta} = -2\sum_{i=1}^{n}(Y_i - \beta X_i)X_i = 0$$

$$\sum_{i=1}^{n}(Y_i - \beta_i X_i)X_i = 0$$

$$\sum_{i=1}^{n} X_i Y_i - \sum_{i=1}^{n} \beta X_i^2 = 0$$

$$b = \widehat{\beta} = \frac{\sum_{i=1}^{n} X_i Y_i}{\sum_{i=1}^{n} X_i^2}.$$

(b) Now that you have the estimate, find its variance.

$$Var(b) = Var\left(\frac{\sum_{i=1}^{n} X_i Y_i}{\sum_{i=1}^{n} X_i^2}\right) = \sum_{i=1}^{n}\left(\frac{X_i}{\sum_{i=1}^{n} X_i^2}\right)^2 \sigma^2 = \frac{\sigma^2}{\sum_{i=1}^{n} X_i^2}.$$

11.1.3 Model Assumptions and MS(E)

So far we said nothing about the probability distribution. We have *no basis* for running statistical tests of constructing confidence intervals. To perform these tasks, we require some *distribution assumptions.* The assumptions are:

1. ϵ_i is a random variable with mean zero and variance σ^2. That is $E(\epsilon_i) = 0$, and $Var(\epsilon_i) = \sigma^2$. ϵ_i and ϵ_j are uncorrelated.

2. $E(y_i) = \beta_0 + \beta_1 x_i$, and $Var(y_i) = \sigma^2$.
3. ϵ_i has a normal distribution.

In Chapter 6 of the text book, we will learn how to check the validity of these assumptions. In Chapter 5 of the text book, we will use these to construct confidence intervals. In building confidence intervals, we will require a point estimate of the underlying variance σ^2. It can be shown that $E(SSE) = (n-2)\sigma^2$ using assumptions 1 and 2. Hence, a point estimate for σ^2 is $s^2 = \frac{SS(E)}{n-2} = MS(E)$ called the *mean square error.* The *residual* is the difference between the observed value of y and the predicted value of y.

A FACT: $w_1, w_2, ..., w_k$ are random variables. $c_1, c_2, ..., c_k$ are constants. Then,

$$Var\left(\sum_{i=1}^{k} c_i w_i\right) = \sum_{i=1}^{k} c_i^2 Var(w_i) + \sum_{i=1}^{k}\sum_{j=1}^{k} c_i c_j Cov(w_i, w_j), i \neq j.$$

If the w_i's are uncorrelated , then

$$Var\left(\sum_{i=1}^{k} c_i w_i\right) = \sum_{i=1}^{k} c_i^2 Var(w_i)$$

since the covariances are zero. If in addition, $c_i = \frac{1}{k}, \forall i$ and $Var(w_i) = \sigma^2, \forall i$, then

$$Var\left(\sum_{i=1}^{k} c_i w_i\right) = \sum_{i=1}^{k} \left(\frac{1}{k}\right)^2 \sigma^2 = \frac{\sigma^2}{k}.$$

11.1.4 Inference in Simple Linear Regression

Inference for β. The estimate for β_1 is

$$b_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})y_i}{\sum_{i=1}^{n}(x_i - \bar{x})^2} = \sum_{i=1}^{n} c_i w_i$$

where $c_i = \frac{x_i - \bar{x}}{\sum(x_i - \bar{x})^2}$ and $w_i = y_i$. The variance of this estimate is

$$Var(b_1) = Var\left(\sum_{i=1}^{n} c_i w_i\right) = \sum_{i=1}^{n} c_i^2 Var(w_i) + \sum\sum Cov(w_i, w_j) = \sum_{i=1}^{n} c_i^2 \sigma^2 + 0 = \sum_{i=1}^{n} c_i \sigma^2 =$$

$$\frac{\sum_{i=1}^{n}(x_i - \bar{x})^2}{\left[\sum_{i=1}^{n}(x_i - \bar{x})^2\right]^2}\sigma^2 = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}.$$

The standard deviation is $SD(b_1) = \sigma\sqrt{c_{11}}$. So the estimated standard deviation of b_1 is

$$s\sqrt{c_{11}} = \frac{s}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}}.$$

This result is called the *standard error* of b_1. Our $(1-\alpha)100\%$ confidence interval for β_1 is $b_1 \pm t_{\alpha/2}(n-2)SE(b_1) = b_1 \pm t_{\alpha/2}(n-2)s\sqrt{c_{11}}$. That appears at the bottom of page 145 in the text book.

Example: The computer repair handout. $15.51 \pm 1.782(0.505)$ the degrees of freedom is 12. A 90% confidence interval is $15.51 \pm 0.90 = [14.61, 16.41]$. The test for β_1 is as follow: $H_0 : \beta_1 = \beta_1^0$ vs $H_1 : \beta_1 \neq \beta_1^0$. Reject H_0 if $t = b_1 = \frac{\beta_1^0}{SE(b_1)} > t_{\alpha/2}(n-2)$ or $t = b_1 = \frac{\beta_1^0}{SE(b_1)} < t_{\alpha/2}(n-2)$. The most widely used and most important application of the test is $H_0 : \beta_1 = 0$ vs $H_1 : \beta_1 \neq 0$. Lets test β_1 of the computer repair with $\alpha = 0.05$. Then, $t_{\alpha/2}(n-2) = t_{0.025}(12) = 2.179$. Reject H_0 if the test statistic $t > 2.179$ or $t < -2.179$. $t = \frac{b_1}{SE(b_1)} = \frac{15.509}{0.505} = 30.711 > 2.179$. Therefore, reject H_0. Conclude that $\beta_1 \neq 0$. x does contribute to the prediction of y.

11.1.5 Inference for β_0

Using reasoning similar to β_1, we can derive the following quantities and expressions for b_0.

$$Var(b_0) = \sigma^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^n (x_i - \bar{x})^2} \right] = \sigma^2 c_{00}.$$

$SD(b_0) = \sigma^2 \sqrt{c_{00}}$. The standard error for b_0 is $s\sqrt{c_{00}}$. A $(1-\alpha)100\%$ confidence interval for b_0 is $b_0 \pm t_{\alpha/2}(n-2)s\sqrt{c_{00}}$. The test statistic for testing $H_0 : \beta_0 = 0$ vs $H_1 : \beta_0 \neq 0$ is $t = \frac{b_0}{SE(b_0)}$. Reject H_0 if $t > t_{\alpha/2}(n-2)$ or $t < -t_{\alpha/2}(n-2)$.

11.1.6 Inference for y

Estimate the mean value of y at a given x. The average of y at $x = x_0$ is $\mu_0 = \beta_0 + \beta_1 x_0$. The estimate for μ_0 is $\mu_0 = \widehat{y}_0 = b_0 + b_1 x_0 = \bar{y} + b_1(x_0 - \bar{x})$. The variance of the estimation is

$$Var(\widehat{y}_0) = Var(\bar{y} + b_1(x_0 - \bar{x})) = Var(\bar{y}) + Var(b_1(x_0 - \bar{x})) + 2Cov(\bar{y}, b_1(x_0 - \bar{x})) =$$

$$Var(\bar{y}) + (x_0 - \bar{x})^2 Var(b_1) + 2(x_0 - \bar{x})Cov(\bar{y}, b_1) = \frac{\sigma^2}{n} + (x_0 - \bar{x})^2 \sigma^2 c_{11} = \sigma^2 \left(\frac{1}{n} + (x_0 - \bar{x})c_{11} \right) =$$

$$\sigma^2 \left(\frac{1}{n} + \frac{(x_0 - \bar{x})^2}{\sum (x_i - \bar{x})^2} \right) = \sigma^2 h_{00}.$$

From that, we get the standard deviation $\widehat{y}_0 = \sigma\sqrt{h_{00}}$ and the standard error $s\sqrt{h_{00}}$. The $(1-\alpha)100\%$ confidence interval for μ_0 is

$$\widehat{y}_0 \pm t_{\alpha/2}(n-2)s\sqrt{h_{00}} = [\bar{y} + b_1(x_0 - \bar{x}] \pm t_{\alpha/2}(n-2)s\sqrt{\frac{1}{n} + \frac{(x_0 - \bar{x})^2}{\sum (x_i - \bar{x})^2}}.$$

1. The smallest standard error is when $x_0 = \bar{x}$. The further you go from the center of the data, the worse the estimate performs.
2. By changing x_0, we can produce confidence intervals for μ_0 at every possible x. This gives confidence bands. See page 169 of the text book.
3. Confidence bands are not widely used in practice.

To predict a *new* y at $x = x_0$, we have the estimate $\widehat{y}_0 = b_0 + b_1 x_0 = \bar{y} + b_1(x_0 - \bar{x})$. The standard error is $s\sqrt{1 + h_{00}} =$

$$s\sqrt{1 + \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{\sum (x_i - \bar{x})^2}}.$$

The confidence interval is $\widehat{y}_0 \pm t_{\alpha/2}(n-2)s\sqrt{1 + h_{00}}$.

11.1.7 Simple Coefficients of Determination and Correlation

$$SS(TOTAL) = SS(MODEL) + SS(E).$$

SS(MODEL) is also called SS(REGRESSION).

$$\sum_{i=1}^n (y_i - \bar{y})^2 = \sum_{i=1}^n (\bar{y}_i - \bar{y})^2 + \sum_{i=1}^n (y_i - \widehat{y}_i)^2.$$

$$R^2 = \frac{SS(MODEL)}{SS(TOTAL)} = 1 - \frac{SS(E)}{SS(TOTAL)}.$$

11.1.8 An F-Test for Simple Linear Regression

Each of the sums of squares in the identity above has a degrees of freedom associated with it and these are displayed in an ANOVA table.

Source	d.f.	SS	MS
Model	1	SS(MODEL)	SS(MODEL)/1
Error	$n-2$	SS(ERROR)	SS(E)/$(n-2)$
Total	$n-1$	SS(TOTAL)	

A *mean square* is the sum of squares divided by the degrees of freedom. The *F-ratio* provides a test of $H_0 : \beta_1 = 0$ versus $H_1 : \beta_1 \neq 0$. It is given by: $\frac{MS(MODEL)}{MS(E)} = F(MODEL)$. Reject H_0 if $F(MODEL) > F_\alpha(1, n-2)$.

11.1.9 Homework and Answers

1. Problem 5.1 in the text book on pages 196-197 — do by hand and using results from HW1.

5.1a $H_0 : \beta_1 = 0$ versus $H_1 : \beta_1 \neq 0$. $t_{0.025}(5) = 2.571$. The test statistic is

$$t = \frac{b_1}{SE(b_1)} = \frac{4.752111}{\frac{\sqrt{0.21224}}{\sqrt{1.841}}} = 13.996.$$

Since $13.996 > 2.571$, reject H_0. x does contribute to y.

5.1b $H_0 : \beta_0 = 0$ versus $H_1 : \beta_0 \neq 0$. The test statistic is

$$t = \frac{12.34242}{0.461\left(\sqrt{\frac{1}{7} + \frac{(3.081429)^2}{1.841}}\right)} = 12.59.$$

Since $12.59 > 2.571$, reject H_0. For $\alpha = 0.01$, $t_{0.005}(7) = 4.032$. Since $4.032 < 12.59$, we can reject H_0 at a higher confidence level.

5.1c Total variance is given by $\sum_{i=1}^{7}(y_i - \bar{y})^2 = 42.63$. Explained variance is given by $\sum_{i=1}^{7}(\widehat{y}_i - \bar{y})^2 = 41.5674$. Unexplained variance is given by $\sum_{i=1}^{7}(y_i - \widehat{y}_i)^2 = 1.0612$. Then, $r^2 = \frac{41.5674}{42.63} = 0.975$. Then, $r = 0.987$. The r^2 means that the x and y variables have a high tendency to move together in a linear fashion. r^2 is very high. In general, r^2 is the proportion of total variance of y that is explained by the simple linear regression model.

5.1d $s^2 = \frac{SS(E)}{7-2} = \frac{1.0612}{5} = 0.21224$. Then, $s = 0.461$.

5.1e $b_1 \pm t_{0.025}(5)se(b_1) =$

$$4.752111 \pm (2.571)\left(\frac{\sqrt{0.21224}}{\sqrt{1.841}}\right) = 4.75211 \pm 0.873 = (3.88, 5.63).$$

5.1f $b_0 \pm t_{0.025}(5)s\sqrt{c_{00}} =$

$$12.34242 \pm (2.571)(0.461)\sqrt{\frac{1}{7} + \frac{(3.081429)^2}{1.841}} = 12.34242 \pm 2.73 = (9.61, 15.07).$$

5.1g $\bar{y} + b_1(x_0 - \bar{x}) \pm t_{0.025}(5)s\sqrt{h_{00}} = 27.787 \pm (2.571)(0.461)\sqrt{\frac{1}{7} + \frac{0.02842}{1.841}} = 27.787 \pm 0.472 = (27.315, 28.259)$.

5.1h $\widehat{y}_0 \pm t_{0.025}(5)s\sqrt{1 + h_{00}} = 27.787 \pm (2.571)(0.461)\sqrt{1 + \frac{1}{7} + \frac{0.02842}{1.841}} = 27.787 \pm 1.276 = (26.511, 29.063)$.

5.1i $F(MODEL) = \frac{MS(MODEL)}{MS(E)}$. $SS(MODEL)41.5674$. $MS(MODEL) = \frac{41.5674}{1}$. $F(MODEL) = \frac{\frac{41.5674}{1.0612}}{5} = 195.851$. $H_0 : \beta_1 = 0$ versus $H_1 : \beta_1 \neq 0$. $F_{0.05}(1,5) = 6.61$. Reject H_0.

2. Problem 5.3 on page 197 of the text book — use SAS to obtain as many of the requested calculations as you can.

5.3a $H_0 : \beta_1 = 0$ versus $H_1 : \beta_1 \neq 0$. $t_{\alpha/2}(n-2) = t_{0.025}(28) = 2.048$. The test statistic is $t = \frac{b_1}{se(b_1)} = \frac{2.665214}{0.25849959} = 10.31$. Since $10.31 > 2.048$, reject H_0.

5.3b $b_1 \pm t_{0.025}(28)se(b_1) = 2.665 \pm (2.048)(0.25849959) = 2.665 \pm 0.529 = (2.136, 3.194)$.

5.3e $\widehat{\mu}_0 = b_0 + b_1 x_0 = 7.814 + (2.665)(0.1) = 8.08$.

5.3f $\widehat{\mu}_0 \pm t_{0.025}(28)s\sqrt{h_{00}} = 8.08 \pm (2.048)(0.31656)\sqrt{0.041848}$. Here $h_{00} = \frac{1}{30} + \frac{(0.1-0.213)^2}{1.49967} = 0.041848$. Then, $8.08 \pm 0.133 = (7.947, 8.213)$.

5.3g $\widehat{y}_0 = 8.08 + (2.665)(.1) = 8.3465$.

5.3h $\widehat{y}_0 \pm t_{0.025}(28)s\sqrt{1+h_{00}} = 8.08 \pm (2.048)(0.31656)\sqrt{1.041848} = 8.08 \pm 0.662 = (7.418, 8.742)$.

5.3i $F(MODEL) = \frac{MS(MODEL)}{MS(E)} = \frac{10.65268}{0.10021} = 106.303$.

5.3j $H_0 : \beta_1 = 0$ versus $H_1 : \beta_1 \neq 0$. $F_{0.05}(1,28) = 4.2$. Since $106.303 > 4.2$, reject H_0.

5.3k Total variance is 13.459. Explained variance is 10.653. Unexplained variance is 2.806. $r^2 = \frac{10.653}{13.459} = 0.792$. Approximately 79% of the total variance in 30 observed samples is explained variance.

3. Prove the following for the simple linear regression model: $\sum_{i=1}^n e_i = 0$. $\sum_{i=1}^n x_i e_i = 0$. $\sum_{i=1}^n \widehat{y}_i e_i = 0$. Starting with the first one:

$$\sum_{i=1}^n e_i = \sum_{i=1}^n y_i - b_0 - b_1 x_i = \sum_{i=1}^n y_i - \bar{y} + b_1\bar{x} - b_1 x_i = n\bar{y} - n\bar{y} + nb_1\bar{x} - nb_1\bar{x} = 0.$$

Starting with the second one:

$$\sum_{i=1}^n x_i e_i = \sum_{i=1}^n x_i[y_i - \bar{y} + b_1\bar{x} - b_1 x_i] = \sum_{i=1}^n x_i y_i - \bar{y}x_i + b_1\bar{x}x_i - b_1 x_i^2 =$$

$$\sum_{i=1}^n x_i y_i - \frac{1}{n}\sum_{i=1}^n yi \sum_{i=1}^n x_i + \frac{b_1}{n}\left(\sum_{i=1}^n x_i\right)^2 - b_1\sum_{i=1}^n x_i^2.$$

Expand on b_1 to get zero.

11.1.10 An F-Test of Lack of Fit

The i-th residual is $\epsilon_i = y_i - \widehat{y}_i$. Let $\eta_i = E(y_i)$. If the model is correct, then $\eta_i = \mu_i = \beta_0 + \beta_1 x_1$. Rewrite ϵ_i as

$$\epsilon_i = (y_i - \widehat{y}_i) - E(y_i - \widehat{y}_i) + E(y_i - \widehat{y}_i) = [y_i - \widehat{y}_i - E(y_i - \widehat{y}_i)] + \overbrace{[\eta_i - E(y_i)]}^{\text{biasness}}.$$

The lack-of-fit test assesses whether or not the bias terms are zero. It requires multiple observations at some x values.

Suppose we have data y_{11}, y_{12}, y_{1n_1} at $x = x_1$, y_{21}, y_{22}, y_{2n_2} measurements at $x = x_2$ and so on. Then,

$$SS(E) = \sum_{L=1}^m \sum_{k=1}^{n_L} (y_{Lk} - \bar{y}_L)^2 = \overbrace{\sum_{L=1}^m \sum_{k=1}^{n_L} (y_{Lk} - \bar{y}_L)^2}^{\text{SS(PE)}} + \overbrace{\sum_{L=1}^n n_L(\bar{y}_L - \widehat{y}_L)^2}^{\text{SS(LF)}}$$

where the degrees of freedom for SS(E) are $n-2$, the degrees of freedom for SS(PE) are $n-m$ and the degrees of freedom for SS(LF) are $m-2$. Then,

$$MS(PE) = \frac{SS(PE)}{n-m}, \;\; MS(LF) = \frac{SS(LF)}{m-2}, \;\; F(LF) = \frac{MS(LF)}{MS(PE)}.$$

H_0 : the model fits versus H_1 : model is biased. Reject H_0 if $F(LF) > F_\alpha(m-2, n-m)$.

SAS Code

```
OPTIONS NODATE;
DATA REPAIR;
INPUT N_UNITS MINUTES;
LACKOFIT = N_UNITS;
CARDS;
1 23
2 29
3 49
4 64
4 74
5 87
6 96
6 97
7 109
8 119
9 149
9 145
10 154
10 166
11 162
11 174
12 180
12 176
14 179
16 193
17 193
18 195
18 210
18 198
20 205
;

PROC PLOT;
PLOT MINUTES*N_UNITS;
RUN;

PROC REG;
MODEL MINUTES = N_UNITS;
OUTPUT OUT=NEW P=PRED R=RESID;
RUN;

PROC PLOT;
PLOT MINUTES*N_UNITS='O' PRED*N_UNITS='*'/OVERLAY;
PLOT RESID*N_UNITS='*'/VREF=0;
RUN;
```

```
PROC UNIVARIATE NORMAL PLOT;
VAR RESID;
RUN;

PROC GLM DATA=REPAIR;
CLASS LACKOFIT;
MODEL MINUTES = N_UNITS LACKOFIT;
RUN;
```

The lack-of-fit test is performed in SAS by creating a variable that is identical to the independent variable, and declaring it a CLASS variable in PROC GLM. The class variable is then placed as the last term in the model statement and the regression is run. PROC GLM is another proc for fitting linear models, which we use for this application because PROC REG does not have a class statement for creating grouping variables.

11.2 Assumptions Behind Regression

The 3 assumptions behind regression make certain statements about the $\epsilon_i's$ which we wish to evaluate. We check these assumptions by inspecting the *residuals*, $\epsilon_i = y_i - \widehat{y}_i, i = 1, 2, ..., n$. If the model(including the assumptions) is correct, then the residuals should behave in a way consistent with the model. The assumptions are:

1. Variance of the residuals is constant.
2. The measurements are uncorrelated.
3. The measurements are normally distributed.

There are two methods for assessing this behavior: 1) plots and 2) statistics for isolating unusual residuals. Plots include:

1. Plot the residuals versus x_i to verify assumption 1.
2. Plot the residuals versus $\widehat{y}_i$ to verify assumption 1.
3. Plot the residuals versus time/space ordering variable to verify assumption 2.
4. Use a scatterplot, box plot, or a stem-leaf plot to verify assumption 3.

11.2.1 Shapiro-Wilks Test of Normality

The hypotheses are H_0 : data comes from a normal distribution versus H_1 : data does not come from a normal distribution. The test statistic is

$$W = \frac{\left(\sum_{i=1}^{n} a_i x_{(i)}\right)^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2},$$

when given a random sample $x_1, x_2, ..., x_n$. The numerator is the best estimate of the standard deviation based on a linear combination of the order statistics. a_i and the reject points can be found in the original paper in Biometrika(1965), volume 52. SAS uses this test for any $n \leq 2000$ data points. For $n > 2000$ SAS uses Kolmogorov's statistic.

11.2.2 Lack of Independence

Plot ϵ_i versus time/space to see if the data is ordered. Positive correlation looks at positive/negative runs of numbers. Plot the residuals against time/space variable. Look for non-random patterns.

Strategy 1: Evaluate runs of positive and negative signs. Long runs indicate positive correlation. Short runs indicate negative correlation.

Strategy 2: The Durbin-Watson test. The Durbin-Watson test looks for correlation arising from the model $E_\mu = \rho\epsilon_{\mu-1} + z_\mu$, where $z_\mu \sim N(0, \sigma^2)$ independent of the $\epsilon's$. For this model, lag-s correlation $= \rho^s, |\rho| < 1$. $H_0 : \rho = 0$ versus $H_1 : \rho < 0$ or $H_1 : \rho > 0$ or $H_1 : \rho \neq 0$. The test statistic is

$$d = \frac{\sum_{u=2}^{n}(\epsilon_u - \epsilon_{u-1})^2}{\sum_{u=2}^{n}\epsilon_u^2}.$$

See page 239 of the text book on how to determine the rejection region.

SAS Code

```
*SEE PAGE 240 OF THE TEXT BOOK;

DATA PRICEY;
INPUT T Y X;
LABEL T = 'TIME'
Y = 'DEMAND'
X = 'PRICE DIFFERENCE';
CARDS;
1 7.38 -0.05
2 8.51 0.25
...
30 9.26 0.55;

PROC PLOT;
PLOT Y*X;
RUN;

PROC REG;
MODEL Y = X/DW;
OUTPUT OUT=NEW P=PREDICTED R=RESID;
RUN;

DATA NEW1;
SET NEW;
SIGNRES = SIGN(RESID);

PROC PRINT L;
RUN;

PROC PLOT;
PLOT Y*X='O' PREDICTED*X='*'/OVERLAY;
PLOT RESID*X/VREF=0;
RUN;
```

11.2.3 Sign Testing for Checking Assumption 2

Data is in order according to some time or space variable. Examine the ordered residuals. Specifically, look at the sequence of signs they produce. Properties of the sequence of signs:

1. Few runs means positive correlation.

2. Many runs means negative correlation.

3. Moderate runs means uncorrelated.

The *sign test* test the number of runs as a way of testing for correlation. Let u be the number of runs, n_1 be the number of positive signs, and n_2 be the number of negative signs. The tables in the book report the cdf of u for given n_1, n_2. H_0 : no correlation versus H_1 : positive correlation. Reject if $P(U \leq u)$ is small. H_1 : negative correlation. Reject if $P(U \geq u)$ is small. Small is less than α or your p-value.

Example: Test for positive correlation with $n_1 = 9$, $n_2 = 7$ and $u = 5$. p-value $= P(U \leq 5) = 0.035$. Thus, reject H_0 at $\alpha = 0.05$. Conclude that there is positive correlation.

Example: Test the following sequence for negative correlation: $+, -, +, -, +, +, -, +, -, -, -, +, +, -, +, +$. Here $n_1 = 9, n_2 = 7, u = 11$. The p-value is $P(U \geq u) = 1 - P(U \leq 10) = 1 - 0.806 = 0.194$. Fail to reject H_0.

For n_1, n_2 outside the range of the tables, there is a normal approximation. μ = mean number of runs $= \frac{2n_1n_2}{n_1+n_2} + 1$. σ^2 = variance of the number of runs $= \frac{2n_2n_2(2n_1n_2-n_1-n_2)}{(n_1+n_2)^2(n_1+n_2-1)}$. The test statistic is $z = \frac{u-\mu\pm 0.5}{\sigma}$. Use $+0.5$ for positive correlation and -0.5 for negative correlation.

Example: Test for negative correlation when $n_1 = 12, n_2 = 18$ and $u = 17$. $\mu = \frac{2(12)(18)}{12+18} + 1 = 15.4$. $\sigma^2 = \frac{2(12)(18)[2(12)(18)-12-18)]}{(12+18)^2(12+18-1)} = 6.6538$. Then, $z = \frac{17-15.4-0.5}{\sqrt{6.6538}} = 0.43$. Fail to reject H_0.

11.2.4 Homework

1. Problem 6.1 on page 252 of the text book. Omit part (d). Use SAS to get these results. Write your interpretations on the printed listing.

```
* hw 4;
* Roger Goodwin;
* Stat 537;
* Due Thursday, October 3, 1996;
*;
*;
data gpasal;
 input gpa salary;
 cards;
3.26 28.2
2.60 24.8
3.35 27.9
2.86 25.3
3.82 30.3
2.21 23.0
3.47 29.4


proc reg;
model salary = gpa;
output out = new p=predictd r=resid;

proc print;

proc plot;
 plot resid*gpa;
```

```
 plot resid*predictd;

proc univariate normal plot;
var resid;

run;
```

2. Repeat (a), (b), (c), and (e) of (1) but for a simple linear regression using the data in problem 4.22(use y and x_2).

```
* hw 4;
* Roger Goodwin;
* Stat 537;
* Due Thursday, October 3, 1996;
*;
*;
data priceage;
 input age price;
 lackofit = age;
 cards;
6 4.5
4 54.9
4 47.0
3 47.0
3 70.0
3 42.5
2 48.0
4 45.5
3 44.0
3 72.0
6 65.0
3 71.0
3 72.0
3 72.0
2 73.5
2 73.0
3 73.5
3 40.3
4 45.0
4 45.0
4 72.5
2 74.0
2 73.0
;


proc reg;
model price = age;
output out = new p=predictd r=resid;

proc print;

proc plot;
 plot resid*age;
```

```
 plot resid*predictd;

proc univariate normal plot;
var resid;

proc glm data=priceage;
class lackofit;
model price=age lackofit;

run;
```

3. Use SAS to calculate the lack-of-fit test for your model in (2).

11.3 Matrix Algebra

A *matrix* is a rectangular array of numbers or symbols. **A** means matrix **A.**

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & -3 \\ 2 & 1 & 7 \\ 4 & -2 & 6 \\ 0 & 0 & 3 \end{pmatrix}$$

is a 4×3 matrix.

$$\beta = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}$$

is a 2×1 matrix. Matrices with 1 row or 1 column are called *row vectors* or *column vectors.* A 1×1 matrix is just an ordinary number, sometimes called a *scalar.* In general, we will discuss Matrices like the following matrix:

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix}$$

a_{ij} is the element in row i, column j.

11.3.1 The Transpose of a Matrix

The *transpose* of the matrix **A** is found by interchanging rows and columns to obtain an $n \times m$ matrix denoted by $\mathbf{A}'$.

$$\mathbf{A}' = \begin{pmatrix} 1 & 2 & 4 & 0 \\ 0 & 1 & -2 & 0 \\ -3 & 7 & 6 & 3 \end{pmatrix}$$

is a 3×4 matrix.

11.3.2 Sums and Differences of Matrices

Define matrix **A** as the same as before. Define the following Matrices:

$$\mathbf{B} = \begin{pmatrix} 1 & 0 \\ -1 & 2 \\ 0 & 1 \end{pmatrix} \quad \mathbf{C} = \begin{pmatrix} 4 & 3 & 0 \\ 2 & 4 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \mathbf{D} = \begin{pmatrix} 4 & 2 & 1 \\ -2 & -1 & -7 \\ 1 & 2 & 0 \end{pmatrix} \quad \mathbf{E} = \begin{pmatrix} 1 & 0.5 & 2 \\ -2 & 3 & 0 \\ 2 & 0 & 3 \end{pmatrix}$$

Then,

$$\mathbf{A} + \mathbf{D} = \begin{pmatrix} 5 & 2 & -2 \\ 0 & 0 & 0 \\ 1 & 0 & 10 \\ 1 & 2 & 3 \end{pmatrix}$$

And,

$$\mathbf{A} - \mathbf{D} = \begin{pmatrix} -3 & -2 & -4 \\ 4 & 2 & 14 \\ 7 & -4 & 2 \\ -1 & -2 & 3 \end{pmatrix}$$

11.3.3 Matrix Multiplication

Two Matrices can be multiplied if they are *conformable.* That is, if the number of columns of the first matrix is the same as the number of rows of the second matrix. Matrix **A** is a 4×3 matrix, matrix **B** is a 3×2 matrix, matrix **C** is a 3×3 matrix, matrix **D** is a 4×3 matrix, and matrix **E** is a 3×3 matrix. We can multiply **AB, AC,** and **AE.** But, we can not multiply **AD, BC,** etc. The element of row i column j of the product is the product of the i-th row of the first matrix with the j-th column of the second matrix.

$$\mathbf{B}'\ \mathbf{C} = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 2 & 1 \end{pmatrix} \begin{pmatrix} 4 & 3 & 0 \\ 2 & 4 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 4\text{-}2{+}0 & 3\text{-}4{+}0 & 0{+}0{+}0 \\ 0{+}4{+}0 & 0{+}8{+}0 & 0{+}0{+}1 \end{pmatrix} = \begin{pmatrix} 2 & -1 & 0 \\ 4 & 8 & 1 \end{pmatrix}.$$

11.3.4 The Identity Matrix and Inverses

The identity matrix **I** of order n is an $n \times n$ matrix with 1's on the diagonal and 0's elsewhere. An example of a 3×3 identity matrix is

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Multiplication by **I** preserves any matrix. $\mathbf{AI} = \mathbf{A}$ and $\mathbf{IA} = \mathbf{A}$. A *square matrix* is one for which the number of rows is equal to the number of columns. Some square Matrices have inverses. The *inverse* of matrix **A** is another square matrix **B** such that $\mathbf{AB} = \mathbf{I}$. We write $\mathbf{B} = \mathbf{A}^{-1}$.

Consider matrix **E.** 1.5 times the first column plus the second column is equal to the third column. Column three is said to be *linearly dependent* on columns one and two. The columns of a given matrix are said to be linearly dependent if one of its columns can be written as a linear combination of the others. If none of the columns of a given matrix can be written as a linear combination of the other then the columns of the given matrix are said to be *linearly independent.* The maximum number of linearly independent columns of a given matrix is called the *rank* of the matrix. If the rank of the given matrix is equal to the number of columns, then the matrix is said to be of *full column rank.* Square Matrices have inverses iff they are of full rank. A full rank square matrix implies that it is non-singular. If matrix **X** has rank r, then $\mathbf{X}'\mathbf{X}$ also has rank r. If **X** has full column rank, then $\mathbf{X}'\mathbf{X}$ is invertible.

SAS Code

Several options in PROC REG will be demonstrated. The CORRB option gives correlation estimates. The COVB option gives covariance estimates. The I option gives the inverse of $\mathbf{X}'\mathbf{X}$. The XPX option gives the model cross products. The CLM option gives confidence intervals.

```
OPTION LINESIZE = 72;
```

```
DATA REPAIR;
INPUT N_UNITS MINUTES;
N_UNITSQ = N_UNITS**2;
CARDS;
1 23
2 29
...
20 205;

PROC PLOT;
PLOT MINUTES*N_UNITS;
RUN;

PROC REG;
MODEL MINUTES = N_UNITS N_UNITSQ/CORRB COVB I XPX CLM;
OUTPUT OUT=NEW P=PRED R=RESID;
RUN;

PROC PRINT DATA=NEW;
RUN;

PROC PLOT DATA=NEW;
PLOT MINUTES*N_UNITS='O' PRED*N_UNITS='*'/OVERLAY;
PLOT RESID*N_UNITS='*'/VREF=0;
RUN;
```

11.4 Multiple Regression

In order to get a better feeling for the matrix multiplications to follow, we set up the simple linear regression in matrix terms. $y_i = \mu_i + \epsilon_i = \beta_0 + \beta_1 x_i + \epsilon_i, i = 1, 2, ..., n$. $y_1 = \beta_0 + \beta_1 x_1 + \epsilon_1$, $y_2 = \beta_0 + \beta_1 x_2 + \epsilon_2$, ... $y_n = \beta_0 + \beta_1 x_n + \epsilon_n$, Equivalently, $y_1 = \beta_0 x_{10} + \beta_1 x_{11} + \epsilon_1$, $y_2 = \beta_0 x_{20} + \beta_1 x_{21} + \epsilon_2$, ... $y_n = \beta_0 x_{n0} + \beta_1 x_{n1} + \epsilon_n$, where x_{ij} is the i-th measured value for variable x_j, $i = 1, ..., n$ and $j = 0, 1$. The variable x_{i0} always takes the value 1. Let's now write the model in matrix form:

$$\mathbf{Y} = \begin{pmatrix} y_1 \\ y_2 \\ . \\ . \\ . \\ y_n \end{pmatrix}, \quad \mathbf{X} = \begin{pmatrix} x_{10} & x_{11} \\ x_{20} & x_{21} \\ . & . \\ . & . \\ . & . \\ x_{n0} & x_{n1} \end{pmatrix}, \quad \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix}, \quad \mathbf{E} = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ . \\ . \\ . \\ \epsilon_n \end{pmatrix}$$

Then, the model can be written as $\mathbf{Y} = \mathbf{X}\beta + \mathbf{E}.$ If we write

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \\ . \\ . \\ . \\ \mu_n \end{pmatrix}$$

where $\mu_i = E(y_i)$, then $\mu = \mathbf{X}\beta$. Estimate β_0 and β_1 by minimizing

$$\sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2 = \sum_{i=1}^{n} (y_i - \beta_0 x_{i0} - \beta_1 x_{i1})^2 = (\ \mathbf{Y} - \mathbf{X}\beta\ )'(\ \mathbf{Y} - \mathbf{X}\beta\ ).$$

Differentiating with respect to β_0 and setting to zero yields the *normal equations:*

$$nb_0 + \left(\sum_{i=1}^{n} x_{i1}\right) b_1 = \sum_{i=1}^{n} y_i,$$

$$\left(\sum_{i=1}^{n} x_{i1}\right) b_0 + \left(\sum_{i=1}^{n} x_{i1}^2\right) b_1 = \sum_{i=1}^{n} x_{i1} y_i,$$

$$\begin{pmatrix} n & \sum_{i=1}^{n} x_{i1} \\ \sum_{i=1}^{n} x_{i1} & \sum_{i=1}^{n} x_{i1}^2 \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_{i1} y_i \end{pmatrix}.$$

Consider $\mathbf{X}'\mathbf{X} =$

$$\begin{pmatrix} x_{10} & x_{20} & \ldots & x_{n0} \\ x_{11} & x_{21} & \ldots & x_{n1} \end{pmatrix} \begin{pmatrix} x_{10} & x_{11} \\ x_{20} & x_{21} \\ . & . \\ . & . \\ . & . \\ x_{n0} & x_{n1} \end{pmatrix} = \begin{pmatrix} n & \sum_{i=1}^{n} x_{i1} \\ \sum_{i=1}^{n} x_{i1} & \sum_{i=1}^{n} x_{i1}^2 \end{pmatrix}.$$

The *normal equations* in matrix form are $\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{Y}$. The solution to these normal equations is easy. $\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$, provided that $\mathbf{X}$ has full column rank of 2. The estimate of $\mu = \mathbf{X}\beta$ based on our estimate of $\mathbf{b}$ for β is

$$\widehat{\mu} = \mathbf{X}\mathbf{b} = \overbrace{\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'}^{\text{call it } \mathbf{H}}\mathbf{Y} = \mathbf{H}\mathbf{Y} = \widehat{\mathbf{Y}}$$

which is the same matrix but with different variability. Next consider the sums of squares $SS(E) = \sum_{i=1}^{n}(y_i - \widehat{y})^2 = (\mathbf{Y} - \widehat{\mathbf{Y}})'(\mathbf{Y} - \widehat{\mathbf{Y}}) = (\mathbf{Y} - \mathbf{HY})'(\mathbf{Y} - \mathbf{HY}) = [(\mathbf{I} - \mathbf{H})\mathbf{Y}]'[(\mathbf{I} - \mathbf{H})\mathbf{Y}] = \mathbf{Y}'(\mathbf{I} - \mathbf{H})'(\mathbf{I} - \mathbf{H})\mathbf{Y}$. Note that $(\mathbf{I} - \mathbf{H})'(\mathbf{I} - \mathbf{H}) = (\mathbf{I}' - \mathbf{H}')(\mathbf{I} - \mathbf{H}) = (\mathbf{I} - \mathbf{H})(\mathbf{I} - \mathbf{H}) = \mathbf{I} - \mathbf{H} - \mathbf{H} + \mathbf{HH}$; Note that $\mathbf{HH} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' = \mathbf{H}$, which means it is an idempotent matrix. Then, $\mathbf{I} - \mathbf{H} - \mathbf{H} + \mathbf{HH} = \mathbf{I} - \mathbf{H} - \mathbf{H} + \mathbf{H} = \mathbf{I} - \mathbf{H}$. The total sum of squares is $\sum_{i=1}^{n}(y_i - \bar{y})^2$, $\mathbf{Y} - \frac{1}{n}\mathbf{J}_n\mathbf{Y} = (\mathbf{I} - \frac{1}{n}\ \mathbf{J})\mathbf{Y}$. $\sum_{i=1}^{n}(y_i - \bar{y})^2 = [\mathbf{Y} - \frac{1}{n}\mathbf{J}_n\mathbf{Y}]'[\mathbf{Y} - \frac{1}{n}\mathbf{J}_n\mathbf{Y}]$

$$\mathbf{Y}'(\mathbf{I} - \tfrac{1}{n}\ \mathbf{J})'(\mathbf{I} - \tfrac{1}{n}\ \mathbf{J})\mathbf{Y} = \mathbf{Y}'(\mathbf{I} - \tfrac{1}{n}\ \mathbf{J})(\mathbf{I} - \tfrac{1}{n}\ \mathbf{J})\mathbf{Y} = \mathbf{Y}'(\mathbf{I} - \tfrac{1}{n}\ \mathbf{J} - \tfrac{1}{n}\ \mathbf{J} + \tfrac{n}{n^2}\ \mathbf{J})\mathbf{Y} =$$

$$\mathbf{Y}'(\mathbf{I} - \tfrac{1}{n}\ \mathbf{J})\mathbf{Y} = SS(TOTAL).$$

Finally, SS(MODEL) = SS(TOTAL) - SS(E). So,

$$\mathbf{Y}'(\mathbf{I} - \tfrac{1}{n}\ \mathbf{J})\mathbf{Y} - \mathbf{Y}'(\mathbf{I} - \mathbf{H})\mathbf{Y} = \mathbf{Y}'[(\mathbf{I} - \tfrac{1}{n}\ \mathbf{I}) - (\mathbf{I} - \mathbf{H})]\mathbf{Y} = \mathbf{Y}'(\mathbf{H} - \tfrac{1}{n}\ \mathbf{I})\mathbf{Y} = SS(MODEL).$$

The sums are the same in the general case.

SAS Code

This is the multiple regression example using the data on page 306 of the text book. Most of this program is shown on page 346 of the text book.

```
DATA DETR;
INPUT REGION X1 X2 X4 X3 Y;
X3SQ = X3**2;
LABEL REGION = 'SALES REGION'
X1 = 'PRICE FOR FRESH DETERGENT'
X2 = 'AVERAGE INDUSTY PRICE'
X3 = 'ADVERTISING EXPENDITURE($100,000)'
X4 = 'PRICE DIFFERENCE X1-X2'
```

```
X3SQ = 'SQUARE OF X3'
Y = 'DEMAND';
CARDS;
1 3.85 3.8 -0.05 5.50 7.38
2 3.75 4.0 0.25 6.75 8.51
...
30 3.70 4.2 0.55 6.80 9.26
. . . 0.10 6.80 .;

PROC PRINT L;
TITLE 'THE DETERGENT DATA';
TITLE2 'NOTE DATA WITH MISSING VALUES FOR THE DEPENDENT VARIABLE';
TITLE3 'TIS IS NOT USED IN FITTING THE MODEL, BUT REG WILL GIVE Y-HAT';
RUN;

PROC REG DATA=DETR;
MODEL Y = X4 X3 X3SQ/P CLM CLI I XPX COVB;
OUTPUT OUT=ONE R=RESID P=YHAT;
TITLE 'THE DETERGENT DATA';
RUN;

PROC PLOT DATA=ONE;
PLOT RESID*(X4 X3 YHAT)/VREF=0;
TITLE 'RESIDUALS PLOTS FOR THE DETERGENT DATA';
RUN;

PROC UNIVARIATE NORMAL PLOT DATA=ONE;
VAR RESID;
TITLE 'CHECKING DISTRIBUTION OF THE RESIDUALS';
RUN;
```

11.5 Homework and Answers

1. Text, Chapter 7, # 11, 12, 15. Add the following to # 11:

   (a) Calculate $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$, and verify that $\mathbf{H}^2 = \mathbf{H}$ by direct multiplication.

   (b) Assuming that this data for a simple linear regression, calculate b_0 and b_1 using the formulas from Chapter 4, and compare to (d).

7.11a

$$\mathbf{X}'\mathbf{X} = \begin{pmatrix} 6 & 12 \\ 12 & 28 \end{pmatrix}.$$

7.11b

$$(\mathbf{X}'\mathbf{X})^{-1} = \begin{pmatrix} \frac{7}{6} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{4} \end{pmatrix}.$$

7.11c

$$\mathbf{X}'\mathbf{Y} = \begin{pmatrix} 65 \\ 119 \end{pmatrix}.$$

7.11d

$$\begin{pmatrix} \frac{98}{6} \\ -\frac{11}{4} \end{pmatrix}$$

7.11e

$$\mathbf{H} = \begin{pmatrix} 5/12 & 2/12 & -1/12 & 2/12 & -1/12 & 5/12 \\ 1/6 & 1/6 & 1/6 & 1/6 & 1/6 & 1/6 \\ -1/12 & 2/12 & 5/12 & 2/12 & 5/12 & -1/12 \\ 1/6 & 1/6 & 1/6 & 1/6 & 1/6 & 1/6 \\ -1/12 & 2/12 & 5/12 & 2/12 & 5/12 & -1/12 \\ 5/12 & 2/12 & -1/12 & 2/12 & -1/12 & 5/12 \end{pmatrix}$$

7.11f

$$b_1 = \frac{6(10+24+24+28+18+15)-(12)(65)}{6(28)-(12)^2} = -2.75.$$

$$b_0 = \bar{Y} - b_1\bar{X} = \frac{65}{6} + 2.75(2) = 16.333.$$

7.12a

$$\begin{pmatrix} -\frac{1}{12} & \frac{1}{8} \end{pmatrix}.$$

7.12b

$$\begin{pmatrix} -\frac{1}{12} \\ \frac{1}{8} \end{pmatrix}.$$

7.12c

$$\frac{5.5}{24}.$$

7.15a

$$\lambda' = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 0 \end{pmatrix}$$

7.15b

$$\lambda' = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$$

7.15c

$$\lambda' = \begin{pmatrix} 0 & 0 & 1 & 0 & 1 & -1 \end{pmatrix}$$

7.15d

$$\lambda' = \begin{pmatrix} 0 & 2 & 3 & 1 & 0 & 0 \end{pmatrix}$$

7.15e

$$\lambda' = \begin{pmatrix} 0 & -1/3 & -1/3 & -1/3 & 1 & 0 \end{pmatrix}$$

7.15f

$$\lambda' = \begin{pmatrix} 1 & 2 & 5 & 3 & 1 & 6 \end{pmatrix}$$

2. Text, Chapter 8, # 4, 23, 24.

4b

Source	d.f.	SS	MS	F
Model	2	25.462472	12.731236	229.37
Error	5	0.277528	0.0555056	
Total	7	25.74		

4c

$$s = \sqrt{\frac{SS(E)}{5}} = \sqrt{0.0555056} = .236.$$

$$R^2 = \frac{SS(MODEL)}{SS(TOTAL)} = \frac{25.462472}{25.74} = 0.989.$$

$R = 0.995$. The proportion of explained variance in the model to the overall variation is 0.989. This is highly significant.

4d $H_0 : \beta_0 = 0$ versus $H_1 : \beta_0 \neq 0$. $\alpha = 0.05$. $t_{0.025}(5) = 2.571$. The test statistic is

$$t = \left|\frac{b_0}{s\sqrt{c_{00}}}\right| = \frac{12.917034}{0.5492} = 23.52.$$

Since $23.52 > 2.571$, reject H_0. For $\alpha = 0.01$, $t_{0.005}(5) = 4.032$. Reject H_0 again. The line probably does not pass thru the origin.

4e $t = \left|\frac{b_1}{s\sqrt{c_{11}}}\right| = \left|\frac{-0.087064}{0.009035063}\right| = 9.636$. $H_0 : \beta_1 = 0$ versus $H_1 : \beta_1 \neq 0$. Since $9.636 > 4.032$, reject H_0. Changes in x_1 do relate to changes in y. For $x_2 : t = \left|\frac{b_2}{s\sqrt{c_{22}}}\right| = \frac{0.090221}{0.014122} = 6.389$. $H_0 : \beta_2 = 0$ versus $H_1 : \beta_2 \neq 0$. Since $6.389 > 4.032$, reject H_0. Changes in x_2 do relate to changes in y.

4f In general, the confidence interval is given by $b_j \pm t_{\alpha/2}(n-k)s\sqrt{c_{jj}}, j = 0, 1, 2$. For $\beta_0 : b_0 \pm t_{0.025}(5)s\sqrt{c_{00}} = 12.917034 \pm (2.571)(0.5492) = 12.917034 \pm 1.412 = (11.505, 14.329)$. For $\beta_1 : b_1 \pm t_{0.025}(5)s\sqrt{c_{11}} = -0.087064 \pm (2.571)(0.009035063) = -0.087064 \pm 0.02323 = (-0.110, -0.064)$. For $\beta_2 : b_2 \pm t_{0.025}(5)s\sqrt{c_{22}} = 0.090221 \pm (2.571)(0.014122) = 0.090221 \pm 0.036308 = (0.054, 0.127)$. We can be 95% confident that β_0 is in the interval given. We can be 95% confident that β_1 is in the interval given. Finally, we can be 95% confident that β_2 is in the interval given.

4f $x_{01} = 40$ and $x_{02} = 10$. $y_0 = \beta_0 + \beta_1 x_{01} + \beta_2 x_{02}$, $y_0 = 12.917034 - 0.087064x_{01} + 0.090221x_{02}$, $y_0 = 12.917034 - 0.087064(40) + 0.090221(10)$, $\widehat{y}_0 = 10.34$.

4h $\widehat{\mu}_0 \pm t_{0.005}(5)s\sqrt{h_{00}} = \widehat{\mu}_0 \pm (4.032)(0.109411) = 10.34 \pm 0.441 = (9.899, 10.781)$. The population mean μ_0 is probably in the interval (9.899, 10.781) with 99% confidence.

4i $\widehat{y}_0 \pm t_{0.005}(5)\sqrt{1+h_{00}} = s\sqrt{1+h_{00}} = (0.236)(1.102239) = 0.26013$. Then $10.34 \pm (4.032)(0.26013) = 10.34 \pm 1.05 = (9.291, 11.39)$.

Use SAS for 8.23 and 8.24. Otherwise perform calculations with a hand calculator. The SAS code for both problems is as follow:

```
DATA CREST;
INPUT X1 X2 X3 Y;
X1SQ = X1*X1;
X2SQ = X2*X2;
X3SQ = X3*X3;
LABEL X1 = 'BUDGET'
X2 = 'RATIO'
X3 = 'PERSONAL INCOME'
X1SQ = 'X1 SQUARED'
X2SQ = 'X2 SQUARED'
X2SQ = 'X3 SQUARED';
```

```
CARDS;
16300 1.25 547600000000 1050000
...
28000 1.56 1821700000000 245000
;

*REDUCED MODEL
PROC REG DATA=CREST;
MODEL Y = X1-X3/P CLM CLI I XPX COVB;
OUTPUT OUT=NEW R=RESID P=PRED;
RUN;

PROC PLOT DATA=NEW;
PLOT RESID*(X1 X2 X3 PRED)/VREF=0;
TITLE 'RESIDUALS PLOTS FOR CREST DATA';

PROC UNIVARIATE PLOT NORMAL;
VAR RESID;
RUN;

*COMPLETE MODEL;
PROC REG DATA = CREST;
MODEL Y = X1-X3 X1SQ X2SQ X3SQ/P CLM CLI I XPX COVB;
OUTPUT OUT=NEW2 R=RESID P=PRED;
RUN;

PROC PLOT DATA=NEW2;
PLOT RESID(X1 X2 X3)/VREF=0;
RUN;

PROC UNIVARIATE PLOT NORMAL;
VAR RESID;
RUN;
```

11.6 Test #1

Most of the answers to this test can be found in the notes.

1. For the general multiple regression setting,

   (a) Write down the model, discussing the role of each matrix or vector with an explanation of the concept it represents, and stating the corresponding dimensions.

   (b) Write down the normal equations and their solutions.

   (c) Write down the assumptions 1 – 3.

2. We learned several techniques, for assessing the adequacy of the regression model and the correctness of the assumptions, that involve plotting the residuals. Briefly explain three of these plots, including sketches to show what types of behavior can be ascertained from them.

3. Here is a small dataset with measurements on two variables x and y :

y	x
1	3
1	5
2	6
3	4
4	10
4	6
6	8

(a) You want to fit a simple linear regression of y on x. Write down the vectors $\mathbf{Y}$ and β, and the matrix $\mathbf{X}$, that would be used to write the model in matrix notation. Also find $\mathbf{X}'\mathbf{Y}$ and $\mathbf{X}'\mathbf{X}$.

(b) Find the solution to the normal equations(you need not use the matrix formulation if you do not wish to).

(c) Test the hypothesis $H_0 : \beta_1 = 0$ that there is no regression.

4. Dr. Morgan gave out a SAS printout and asked to identify certain parts of it. This has been intentionally omitted.

11.7 The General Linear Regression Model

Our goal is to use an arbitrary number of independent variables to predict y. Our initial model is still $y_i = \mu_i + \epsilon_i$, and we will model the mean μ_i of y_i at given values of x's with a linear function of the x's. Let x_{i1} be the i-th value of the independent variable x_1, x_{i2} be the i-th value of the independent variable x_2, and so on. Our model is

$$y_i = \mu_i + \epsilon_i = \overbrace{\beta_0 x_{i0} + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}}^{\text{model for } \mu_i} + \epsilon_i, i = 1, ..., n.$$

Define the following Matrices:

$$\mathbf{Y} = \begin{pmatrix} y_1 \\ y_2 \\ . \\ . \\ . \\ y_n \end{pmatrix}, \quad \mathbf{X} = \begin{pmatrix} x_{10} & x_{11} & x_{12} & \dots & x_{1p} \\ x_{20} & x_{21} & x_{22} & \dots & x_{2p} \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ x_{n0} & x_{n1} & x_{n2} & \dots & x_{np} \end{pmatrix}, \quad \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ . \\ . \\ . \\ \beta_p \end{pmatrix} \quad \mathbf{E} = \begin{pmatrix} \epsilon_0 \\ \epsilon_1 \\ \epsilon_2 \\ . \\ . \\ . \\ \epsilon_n \end{pmatrix}.$$

Then the model in matrix terms is $\mathbf{Y} = \mathbf{X}\ \beta + \mathbf{E}$.

11.7.1 Special Cases

1. Simple linear regression with one independent variable. The model is $y_i = \beta_0 x_{i0} + \beta_1 x_{i1} + \epsilon_i$.

2. Quadratic regression where there are two independent variables, $p = 2$, but the second variable is the square of the first. $x_{i2} = x_{i1}^2$. Then, the model is $y_i = \beta_0 x_{i0} + \beta_1 x_{i1} + \beta_2 x_{i1}^2 + \epsilon_i$. Note that linear refers to the combination of independent variables.

3. p-th order polynomial relation on one independent variable. $x_{i2} = x_{i1}^2$, $x_{i3} = x_{i1}^3, \ldots\ x_{ip} = x_{i1}^p$. The model is $y_i = \beta_0 x_{i0} + \beta_1 x_{i1} + \beta_2 x_{i1}^2 + \cdots + \beta_p x_{i1}^p + \epsilon_i$.

4. 2-dimensional quadratic response surface. The model is $y_i = \beta_0 x_{i0} + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i1} x_{i2} + \beta_4 x_{i1}^2 + \beta_5 x_{i2}^2 + \epsilon_i$.

11.7.2 Assumptions, Standard Errors, and Residual Analysis

As with simple linear regression, we have 3 assumptions.

1. For any fixed values $(x_{i1}, x_{i2}, ..., x_{ip}$ of independent variables $x_1, ..., x_p$, the response y_i has the same variance σ^2.

2. Any 2 values of the response, y_i and y_i' are uncorrelated i.e. $Cov(y_i, y_i') = 0$.

3. The distribution of the population potential values for the response at any given values $x_{i1}, ..., x_{ip}$ of the independent variables $x_1, ..., x_p$ is normal i.e. $y_i \sim N(\mu_i, \sigma^2)$ where μ_i is the mean of that population.

The 3 assumptions describe the random component of our model. The fixed component is the model for μ_i where $\mu_i = \beta_0 x_{i0} + \beta_1 x_{i1} + \cdots + \beta_p x_{ip}$. We estimate μ_i by estimating the β's. The point estimate of σ^2 is $MS(E) = s^2 = \frac{SS(E)}{n-k}$, where k is the number of β's which is $p+1$. $SS(E) = \sum_{i=1}^{n}(y_i - \widehat{y})^2 = \mathbf{Y}'(\mathbf{I}\text{ - }\mathbf{H})\mathbf{Y}$. Hence, a point estimate of the *standard error* is $s = \sqrt{\frac{SS(E)}{n-k}}$. The SS(E) can also be written as $SS(E) = \mathbf{Y}'(\mathbf{I}\text{ - }\mathbf{H})\mathbf{Y} = \mathbf{Y}'\mathbf{Y}\text{ - }\mathbf{Y}'\mathbf{H}\mathbf{Y} = \mathbf{Y}'\mathbf{Y}\text{ - }\mathbf{Y}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \mathbf{Y}'\mathbf{Y} - \mathbf{b}'\mathbf{X}'\mathbf{Y}$.

To check the assumptions, we use the same plots previously covered. The i-th residual is $\epsilon_i = y_i - \widehat{y}_i$.

$$\mathbf{E} = \begin{pmatrix} e_1 \\ e_2 \\ \cdot \\ \cdot \\ \cdot \\ e_n \end{pmatrix} = \begin{pmatrix} y_1 - \widehat{y}_1 \\ y_2 - \widehat{y}_2 \\ \cdot \\ \cdot \\ \cdot \\ y_n - \widehat{y}_n \end{pmatrix} = \mathbf{Y}\text{ - }\mathbf{X}\mathbf{b} = \mathbf{Y}\text{ - }\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \mathbf{Y}\text{ - }\mathbf{H}\mathbf{Y} = (\mathbf{I}\text{ - }\mathbf{H})\mathbf{Y}.$$

11.7.3 Multiple Coefficient of Determination and Correlation

Recall that SS(TOTAL) = SS(MODEL) + SS(E) where SS(TOTAL) is the sum of squares of *total variation,* SS(MODEL) is the sum of squares of *explained variation,* and SS(E) is the sum of squares of *unexplained variation.* We want to get a model that explains as much of the total variation as possible. The proportion of variation explained is $R^2 = \frac{SS(MODEL)}{SS(TOTAL)} = 1 - \frac{SS(E)}{SS(TOTAL)}$ and is called *multiple coefficient of determination.* $R = \sqrt{R^2}$ is called the *multiple correlation coefficient.*

11.7.4 Overall F-Test and the Basic ANOVA Table

The overall test for the regression model tests $H_0 : \beta_1 = \beta_2 = \cdots = \beta_p = 0$ versus H_1 : at least one $\beta \neq 0$. The test statistic is $F(MODEL) = \frac{MS(MODEL)}{MS(E)} = \frac{\frac{SS(MODEL)}{k-1}}{\frac{SS(E)}{n-k}}$, where k is the number of β's in the model. Reject if $F(MODEL) > F_\alpha(k-1, n-k)$. This test is usually presented in an ANOVA Table.

Source	SS	d.f.	MS	F
Model	SS(MODEL)	$k-1$	MS(MODEL)	F(MODEL)
Error	SS(E)	$n-k$	MS(E)	
Total	SS(TOTAL)	$n-1$		

11.7.5 Inference for β_j

To perform a test for β_j, or to construct a confidence interval, we need an estimate and a standard error. The estimate is b_j. It may be shown that variance of b_j is the $(j+1)$st diagonal entry of the matrix $\sigma^2(\mathbf{X}'\mathbf{X})^{-1}$. Write c_{jj} for the $(j+1)$st diagonal element of $(\mathbf{X}'\mathbf{X})^{-1}$. Then, $Var(b_j) = \sigma^2 c_{jj}$. Hence the standard error for b_j is $\sqrt{MS(E)c_{jj}} = s\sqrt{c_{jj}}$. We now get the confidence interval and the test. A $(1-\alpha)100\%$ confidence interval for β_j is $b_j \pm t_{\alpha/2}(n-k)s\sqrt{c_{jj}}$. The test of $H_0 : \beta_j = 0$ versus $H_1 : \beta_j \neq 0$ is reject H_0 if $|t| = \left|\frac{b_j}{s\sqrt{c_{jj}}}\right| > t_{\alpha/2}(n-k)$.

11.7.6 Confidence Intervals and Prediction Intervals

Recall that $\widehat{y}_0 = b_0 + b_1 x_{01} + b_2 x_{02} + \cdots + b_p x_{0p} = \mathbf{b}'\mathbf{X}_0$ where

$$\mathbf{X}_0 = \begin{pmatrix} 1 \\ x_{01} \\ x_{02} \\ . \\ . \\ . \\ x_{0p} \end{pmatrix}.$$

1. The point estimate of $\mu_0 = \beta_0 + \beta_1 x_{01} + \cdots + \beta_p x_{0p}$ is equal to the mean of the population of y's at x_0.
2. The point prediction of $y_0 = \beta_0 + \beta_1 x_{01} + \cdots + \beta_p x_{0p} + \epsilon_0$ is equal to the new value of y at this x_0.

We want a confidence interval for both (1) and (2). Consider (1). We have $\widehat{y}_0 = \mathbf{b}'\mathbf{X}_0$. It can be shown that $Var(\widehat{y}_0) = \sigma^2 \mathbf{X}_0'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}_0$. So if we write $h_{00} = \mathbf{X}_0'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}_0$, then $Var(\widehat{y}_0) = \sigma^2 h_{00}$, and hence the standard error is $s\sqrt{h_{00}}$. Then the $(1-\alpha)100\%$ confidence interval for μ_0 is $\widehat{y}_0 \pm t_{\alpha/2}(n-k)s\sqrt{h_{00}}$. The $(100-\alpha)100\%$ prediction interval for y_0 is $\widehat{y}_0 \pm t_{\alpha/2}(n-k)s\sqrt{1+h_{00}}$.
Suppose we want to estimate the difference in the mean response at two different set of values for the independent variables, say $\mathbf{X}_{0'}, \mathbf{X}_{0''}$. The estimated means at these two vectors are $\widehat{y}_{0'} = \mathbf{X}_{0'}'\mathbf{b}$, and $\widehat{y}_{0''} = \mathbf{X}_{0''}'\mathbf{b}$. So the *estimated difference* is $\widehat{y}_{0'} - \widehat{y}_{0''} = \mathbf{X}_{0'}'\mathbf{b} - \mathbf{X}_{0''}'$bf b. Let $\mathbf{X}_0' = \mathbf{X}_{0'}' - \mathbf{X}_{0''}'$. Then the estimate of the difference in means is $\mathbf{X}_0'\mathbf{b}$. The standard error of this estimate is $s\sqrt{h_{00}}$ where $h_{00} = \mathbf{X}_0'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}_0$. Then, the $(1-\alpha)100\%$ confidence interval is $(\widehat{y}_{0'} - \widehat{y}_{0''}) \pm t_{\alpha/2}(n-k)s\sqrt{h_{00}}$.

11.8 More on Multiple Regression

11.8.1 Interaction

See Example 9.1 on page 388 of the text book.

SAS Code

```
DATA FROZEN;
INPUT X1 X2 Y;
X3= X1*X2;
LABEL X1 = 'RADIO AND TELEVISION EXPENDITURES'
X2 = 'PRINT EXPENDITURES'
X3 = 'X1*X2'
Y = 'SALES VOLUME';
CARDS;
1 1 3.27
1 2 8.38
...
5 5 21.05
4.5 3.5 .;

PROC PLOT;
PLOT Y*X1=X2;
POLT Y*X2=X1;
RUN;

PROC REG;
MODEL Y = X1 X2;
RUN;
```

```
PROC REG;
MODEL Y = X1 X2 X3/P CLM CLI I COVB;
OUTPUT OUT=NEW R=RESID;
RUN;

PROC UNIVARIATE NORMAL PLOT;
VAR RESID;
RUN;
```

11.8.2 Testing Part of a Model

We often encounter the following problem: we have fit a multiple regression model and we want to know if we can reduce it to a simpler model. The appropriate hypothesis to test is $H_0 : \beta_{g+1} = \beta_{g+2} = \cdots = \beta_p = 0$. Consider the following: SS(TOTAL) = SS(MODEL) + SS(E) holds for both models. Furthermore, since both models have the same y_i's, bo have the same SS(TOTAL). So, $SS(TOTAL) = SS(MODEL)_c + SS(E)_c$, where "c" means complete model which is also equivalent to $SS(TOTAL) = SS(MODEL)_r + SS(E)_r$ where "r" means reduced model and obviously $SS(E)_r \geq SS(E)_c$, and $SS(MODEL)_c \geq SS(MODEL)_r$. Define $SS(E)_{drop} = SS(E)_r - SS(E)_c = SS(MODEL)_c - SS(MODEL)_r$ which is the reduction in unexplained variation from going from the reduced model to the complete model. The degrees of freedom of $SS(E)_{drop}$ are $[n - (g + 1)] - [n - (p + 1)] = p - g$. So, $MS(E)_{drop} = \frac{SS(E)_{drop}}{p-g}$. The test we want is based on this statistic.

$$F(x_{g+1}, x_{g+2}, ..., x_p | x_1, x_2, ..., x_g) = \frac{MS(E)_{drop}}{MS(E)_{complete}}.$$

Reject $H_0 : \beta_{g+1} = \beta_{g+2} = \cdots = \beta_p = 0$ if $F > F_\alpha(p - g, n - k)$. The Type I SS is $SS(E)_{drop}$ for putting a variable in the model given that the variables before it are already in the model. Type I SS are order dependent. Type II SS is $SS(E)_{drop}$ for putting this variable in last given all other variables in the model statement are already in the model.

SAS Code

This is the detergent data again. We will fit an interaction term (see pages 397 — 400 in the text book) and demonstrate the use of Type I and Type III sums of squares to test for a reduced model.

```
DATA DETR;
INPUT REGION X1 X2 X4 X3 Y;
X3SQ = X3**2;
X43 = X4*X3;
CARDS;
1 3.85 3.8 -0.05 5.50 7.38
...
30 3.7 4.2 0.55 6.8 9.26
.   .   .  0.10 6.80 .
;

PROC REG DATA=DETR;
MODEL Y = X4 X3 X43 X3SQ/SS1 SS2;
TITLE 'THE FULL MODEL';
RUN;

PROC REG DATA=DETR;
MODEL Y = X4 X3;
TITLE 'THE REDUCED MODEL';
RUN;
```

11.9 Outliers and Influential Observations

Outliers are observations with un-usually large residuals (outlier with respect to y) or with x values far from the other x's(outlier with respect to x). *Influential observations* are those that play a disproportionate role in determining the regression line. Any particular measurement can be both, one or the other, or neither. We consider statistics for identifying such measurements. Here $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}$.

1. The *leverage value* is h_{ii}. This is a method for identifying observations whose x values are outlying. h_{ii} is the i-th diagonal element of $\mathbf{H}$. This is called the leverage of the i-th measurement of $\mathbf{X}_i$. It can be shown that $0 \le h_{ii} \le 1$ and $\sum_{i=1}^{n} h_{ii} = k$. A leverage value is considered large if

   (a) It is substantially larger than other leverage values.
   (b) It is greater than $2\bar{h} = \frac{2k}{n}$.

   Values with high leverage values are potentially influential and bear further investigation.

2. *Studentized residual* is used to detect outliers in y. The calculation of the i-th studentized residual is
$$\frac{e_i}{s\sqrt{1-h_{ii}}}.$$

3. *Difference in fits statistic.* Let $\widehat{y}_{(i)}$ be the predicted value of y_i using the regression equation obtained from all of the data *except* the i-th measurement. $f_i = \widehat{y}_i - \widehat{y}_{(i)}$. The difference in fits statistic is f_i divided by its standard error s_{f_i}. It can be shown that the difference in fit is
$$\frac{f_i}{s_{f_i}} = \left(\frac{d_i}{s_{d_i}}\right)\left(\frac{h_{ii}}{1-h_{ii}}\right)^{\frac{1}{2}}$$
where $d_i = y_i - \widehat{y}_{(i)}$. The will tell if the measurement is "drawing the equation to itself." Look for large difference in fits. If it is greater than 2 or greater than $2\sqrt{\frac{p}{n-p}}$ then it is an outlier. Or, look for values much larger than most others.

4. *Cook's distance* is defined as $D_i = (\mathbf{b} - \mathbf{b}^{(i)})'\mathbf{X}'\mathbf{X}(\mathbf{b} - \mathbf{b}^{(i)})$ where $\mathbf{b}^{(i)}$ is the estimate of β with the i-th measurement deleted. It can be shown that
$$D_i = \left(\frac{e_i}{s\sqrt{h_{ii}}}\right)^2\left(\frac{h_{ii}}{1-h_{ii}}\right)\left(\frac{1}{k}\right).$$
It combines the studentized residual with the leverage. It is very similar to the difference in fits statistic. An observation is influential if $D_i > F_{0.5}(k, n-k)$ It is best to just look for large D_i relative to the others with a stem-and-leaf plot.

5. *Difference in estimation of β_j statistic.* Let $g_j^{(i)} = b_j - b_j^{(i)}$. $s_{g_j}^{(i)}$ is the standard error of $g_j^{(i)}$. The difference in fits statistic is
$$\frac{g_j^{(i)}}{s_{g_j}^{(i)}} = \left(\frac{d_i}{s_{d_i}}\right)\left(\frac{t_{ji}}{t_j't_j(1-h_{ii})}\right)$$
where t_{ji} is the (j,i) element of $\mathbf{T} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$. t_j' is row j of $\mathbf{T}$. Absolute values greater than $\frac{2}{n}$ are nominated for further investigation.

6. The *covariance ration* corresponding to the i-th measurement is
$$CVR_i = \frac{(s_i)^{2k}}{(s)^{2k}}\left(\frac{1}{1-h_{ii}}\right)$$
where s_i^2 is s^2 calculated for the model with the i-th measurement deleted. This looks at how the variances and covariances of the b_j's change when the i-th measurement is deleted.

   (a) If $CVR_i > 1 + \frac{3k}{n}$, then eliminating the i-th observation significantly damages the precision of SS least estimates.
   (b) If $CRV_i < 1 - \frac{3k}{n}$, then it enhances precision.

SAS Code

The following data appears in "Procedures and Analysis for Staffing Standards Development: Regression Analysis Handbook" published by the Navy Manpower and Material Analysis Center(1979). The goal is to develop a workable model relating labor hours to a number of available variables. We will try to do this while also examining the data for outliers and influential points. We restrict ourselves to fitting the model for only the small to medium sized hospitals, defined as those with daily patient load below 200.

```
DATA HOSPITAL;
INPUT X1 X2 X3 X4 X5 Y;
IF (X1>199) THEN DELETE;
CARDS;
15.57 2463 479.92 18.0 4.45 566.52
...
510.22 86533 15524 371.6 6.35 18854.45
;

PROC REG DATA=HOSPITAL;
TITLE 'HOSPITAL DATA';
MODEL Y = X1 X2 X3 X4 X5; * NOTE THE LARGE P-VALUES FOR THE
    INDIVIDUAL BETAS, DESPITE THE GOOD
    RSQUARE. OBVIOUSLY THERE IS SOME
    REDUNDANT INFORMATION AMONG THE X'S.
    THIS IS A PROBLEM KNOWN AS
    MULTICOLLINEARITY, WHICH WE WILL STUDY
    IN MORE DETAIL LATER;
RUN;

PROC CORR;
VAR X1-X5; * TO STUDY LINEAR RELATIONSHIPS AMONE
 THE X'S. BASED ON THIS WE THROW OUT
 X2, X3, X4. THIS IS ALSO PART OF THE
 PROBLEM OF VARIABLE SELECTION, ALSO
 TO BE STUDIED IN MORE DETAIL LATER;
RUN;

PROC REG DATA=HOSPITAL;
MODEL Y = X1 X5/R INFLUENCE;
OUTPUT OUT=HOSPRES P=PREDICTED R=RES STUDENT=STUDRES;
RUN;

PROC UNIVARIATE NORMAL PLOT;
VAR STUDRES;
RUN;

PROC PLOT;
PLOT RES*PREDICTED RES*X1 RES*X5/VREF=0;
RUN;

*BASED ON THE ABOVE, WE DELETE TWO
OBSERVATIONS AND STUDY THE EFFECT ON
THE MODEL;

DATA HOSPITAL2;
SET HOSPITAL;
```

```
IF(_N_=2 OR _N_=12) THEN DELETE;

PROC REG DATA=HOSPITAL2;
MODEL Y = X1 X5/R INFLUENCE;
OUTPUT OUT=HOSPRES3 P=PREDICTED R=RES RSTUDENT=STUDRESS;
TITLE 'HOSPITAL DATA: X1 AND X5 ONLY WITH 2 OBS REMOVED';
RUN;

PROC PLOT;
PLOT RES*PREDICTED RES*X1 RES*X5/VREF=0;
RUN;
```

11.10 Multicollinearity(Ill Conditioning)

Recall the normal equations are $(\mathbf{X'X})\mathbf{b} = \mathbf{X'Y}$. The solution is $\mathbf{b} = (\mathbf{X'X})^{-1}\mathbf{X'Y}$. Solving the equations requires that $(\mathbf{X'X})$ be non-singular for which the condition is $det(\mathbf{X'X}) > 0$. If $det(\mathbf{X'X}) = 0$, then $\mathbf{X'X}$ can not be inverted and there are *exact dependencies* among the columns of **X.** That is, among the independent variables one or more can be written as linear combinations of the other which says they are redundant and should be removed from the model. More troublesome is when dependencies hold only approximately in which the determinate is close to zero. From a computational point of view, $\mathbf{X'X}$ is difficult to invert due to round off errors in very small numbers. This is no longer a significant problem with modern computers. However, there are other troubling aspects of *Multicollinearity.*

1. Extreme Multicollinearity can cause least square estimates of the β's to be far from their actual values and/or to have the wrong signs. This is because estimates become highly dependent on the particular x values obtained. Small changes in the x's make large changes in the regression equation.

2. Adding or deleting an independent variable can cause large changes in the regression coefficients.

3. Strong Multicollinearity means there is much overlapping information in the $x's$. Hence, t values of the individual $x's$ are small and is difficult to judge which $x's$ are important.

4. Standard errors tend to be very large when strong Multicollinearity is present.

How do we detect Multicollinearity? One way is to inspect the correlation matrix of the $x's$. High correlation among the variables indicate data overlap. This is a good method but not always sufficient since it just looks at redundancy among pairs of the $x's$. Other informal methods are non-significant t tests based on most of the independent variables but with a significant regression model. Another method is to look for regression coefficients with signs opposite from those expected from previous experience or theory. A formal method is provided by the *variance inflation factor.* Recall that the variance is estimated by the $(j+1)$-st diagonal obtained by $s^2(\mathbf{X'X})^{-1}$. Let $x_1, x_2, ..., x_p$ be the independent variables in the model. It can be shown the $(j+1)$-st diagonal element of $(\mathbf{X'X})^{-1}$ is $c_{jj} = \frac{1}{(1-R_j^2)\sum_{i=1}^{n}(x_{ij}-\bar{x}_j)^2}$ where R_j^2 is the R^2 value for the model predicting x_j from $x_1, x_2, ..., x_{j-1}, x_{j+1}, ..., x_p$. If x_j is totally unrelated to the other independent variables, then $R_j^2 = 0$. If x_j can be perfectly predicted from the other $x's$, then $R_j^2 = 1$. The larger R_j^2, and hence the smaller $1 - R_j^2$, the worst is the Multicollinearity problem and the larger is $s^2(b_j)$. Define the variance inflation factor for b_j as $VIF_j = \frac{1}{1-R_j^2}$. As R_j^2 grows, so does the variance inflation factor. The *average variance inflation factor* is given by $AVIF = \frac{\sum_{j=1}^{p} VIF_j}{p}$. Guidelines for the use of variance inflation factors are

1. If the largest $VIF_j > 10$, then there may be a problem.

2. If AVIF is substantially greater than 1, then there may be a problem.

Partial regression plots look for overlap among the independent variables given a single independent variable.

11.10.1 Partial Leverage Plots

Consider expanding the simple linear model $y = \beta_0 + \beta_1 x_1 + \epsilon$ to $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$. We know that $SS(MODEL)$ using $x_2|x_1$ is equal to $SSMODEL(x_1, x_2) - SSMODEL(x_1)$. That is the sums of squares used to test $H_0 : \beta_2 = 0$ in the full model is the difference in the sums of squares model for the two models. Here we look closely at exactly what is occuring. When we fit the model $y = \beta_0 + \beta_1 x_1 + \epsilon$, we get residuals which for now we call $e_{(2)}$. That is the residuals for the model without x_2. Now, we add x_2 to the model. What can it add to our fit for y?

1. Since some of the variation in the $y's$ has already been explained by x_1, the added contribution of x_2 will be in terms of how well it can explain the as-yet unexplained variation: the residuals $e_{(2)}$.

2. Moreover, any overlapping information between x_1 and x_2 will not help for it is already in the model. Only information in x_2 that is not in x_1 will be of help at this point. What information is this? Fit the model $x_2 = \beta_0' + \beta_1' x_1 + \epsilon'$ and call the residuals from this model $e'_{(2)}$. Then, $e_{(2)}$ is the information in x_2 not found in x_1.

This suggests a plot of $e_{(2)}$ against $e'_{(2)}$. The plot is called the *partial leverage residuals plot.* If the plot shows an approximate straight line, then x_2 will be helpful in explaining y when added to the model already containing x_1. In fact, the slope of the regression of $e_{(2)}$ on $e'_{(2)}$ is the fitted value b_2 for β_2 in the full model $y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$.

SAS Code

This is an illustration of the use of partial regression plots employing the hospital data. Recall that we had previously identified observations 2 and 12 as possibly troublesome. Here we see where they occur in the partial regression plots, then inspect the plots again with observation 2 deleted. We also look at these plots for the full model containing all of x_1 thru x_5, which we know are highly collinear. VIF is demonstrated.

```
DATA HOSPITAL;
INPUT X1 X2 X3 X4 X5 Y;
IF (X1>199) THEN DELETE;
IF (_N_=2 | _N_=12) THEN PROBLEM='*'; ELSE PROBLEM='O';
CARDS;
15.57 2463 479.92 18.0 4.45 566.52
...
510.22 86533 15524 371.6 6.35 18854.45
;
PROC REG DATA=HOSPITAL;
ID PROBLEM;
MODEL Y=X1-X5/PARTIAL VIF;
TITLE 'HOSPITAL DATA: THE FULL MODEL';
RUN;

PROC REG DATA=HOSPITAL;
ID PROBLEM;
MODEL Y=X1 X5/PARTIAL R INFLUENCE;
TITLE 'HOSPITAL DATA: X1 AND X5 ONLY';
RUN;

DATA FEWER;
SET HOSPITAL;
IF _N_=2 THEN DELETE;

PROC REG DATA=FEWER;
IF PROBLEM;
```

```
MODEL Y = X1 X5/PARTIAL R INFLUENCE VIF;
TITLE 'HOSPITAL DATA: X1 AND X5 ONLY WITH OBS. 2 DELETED';
RUN;
```

11.11 Model Building

The *principle of parsimony* suggests models with fewer variables are easier to interpret and are less likely to fit the peculiar features of the present data too closely. Want to balance the models against "good fit:" 1) high R^2, 2) small MS(E), and 3) small prediction intervals.

11.11.1 Some Model Comparison Criteria

One possibility is to try every possible model for the set of $x's$ you have available. With p independent variables, there are 2^p possible models. This is reasonable for small p. But, for large p we need other criteria. We consider R^2, adjusted R^2, MS(E), and C. These are closely related and will typically lead to similar conclusions.

- R^2 is a good first indicator of model fit. But it suffers from the fact that adding new variables can not decrease R^2.
- Adjusted R^2 : Let p be the number of independent variables in the model. Then adjusted R^2 is given by $\left(R^2 - \frac{(k-1)}{n-1}\right)\left(\frac{n-1}{n-k}\right), p = k-1$. Suppose the independent variables are simply lists of random numbers with no relation to y. It can be shown that they will still explain enough variation in y to make $R^2 = \frac{k-1}{n-1}$ on average. So, subtract $\frac{k-1}{n-1}$ from R^2. This will on average make $R^2 = 0$ when the independent variables are unrelated to y. However, this over corrects when the $x's$ are related to y. A perfect fit would give $R^2 = 1$ but the subtraction makes it $1 - \frac{k-1}{n-1} = \frac{n-k}{n-1}$. Hence, multiply by $\frac{n-k}{n-1}$ to get the final formula for adjusted R^2. It can be shown that $MS(E) = (1 - \text{adjusted } R^2)\left(\frac{SS(TOTAL)}{n-1}\right)$. So, if MS(E) decreases, then adjusted R^2 increases.
- Mallow's C_k : Let p be the number of independent variables available. Let k be the number of variables including the intercept in a particular model chosen from those available. $C = \frac{SS(E)}{S_p^2} - (n-2k)$ where SS(E) is the sum of squares due to error for the model chosen with $k-1$ independent variables and S_p^2 is the mean square for error for the model using all p independent variables. It can be shown that if a k variable model does not suffer from lack-of-fit, then $E(C) \approx k$. Adequate models should have C close to k. Models having serious lack-of-fit will have C much bigger than k. In general, we would like

  1. C_k to be small so that SS(E) is small.
  2. C_k be close to k.

  Note: if all p variables are used in the model, then $C_{p+1} = p+1$. Hence, this tells you nothing.
- Press: The deleted residuals (or Press residuals) are defined by $d_i = y_i - \widehat{y}_{(i)} = \frac{e_i}{1-h_{ii}}$. The press statistic is $\sum_{i=1}^n d_i^2 = \sum_{i=1}^n \left(\frac{e_i}{1-h_{ii}}\right)^2$. Large values of Press say the model likely has a fit that too strongly depends on a few measurements. Use Press as one method of comparing several competing models that are being examined in detail.

SAS Code

```
THIS IS THE CREST DATA FROM AN EARLIER ASSIGNMENT. WE ILLUSTRATE
ADJUSTED RSQUARE, ETC, AND SHOW ONE ASPECT OF THE STEPWISE FACILITY;

OPTION LINESIZE = 72 NODATE;
```

```
DATA CREST;
INPUT X1 X2 X3 Y;
X1SQ=X1*X1;
X2SQ=X2*X2;
X2SQ=X3*X3;
LABEL X1 = 'BUDGET'
X2 = 'RATIO'
X3 = 'PERSONAL INCOME'
Y = 'CREST SALES'
X1SQ = 'X1 SQUARED'
X2SQ = 'X2 SQUARED'
X3SQ = 'X3 SQUARED';
CARDS;
16.3 1.25 547.9 105.0
...
28.0 1.56 1821.7 245.0
;

*REDUCED MODEL;
PROC REG DATA=CREST;
MODEL Y = X1-X3/ VIF P INFLUENCE R;
TITLE 'LINEAR REGRESSION ANALYSIS WITH 3 INDEPENDENT VARIABLES';
RUN;

*COMPLETE MODEL;
PROC REG DATA=CREST;
MODEL Y = X1-X3 X1SQ X2SQ X3SQ/VIF P INFLUENCE R;
TITLE 'LINEAR REGRESSION WITH 6 INDEPENDENT VARIABLES';
RUN;

*COMPLETE MODEL;
PROC REG DATA=CREST;
MODEL Y = X1-X3 X1SQ X2SQ X3SQ/SELECTION=STEPWISE INCLUDE=3;
TITLE 'LINEAR REGRESSION ANALYSIS WITH 6 INDEPENDENT VARIABLES';
TITLE2 'USING STEPWISE WITH X1-X3 FORCED INTO THE MODEL';
```

11.11.2 Backwards, Forward, and Stepwise Selection Procedures

- Backward Elimination: operates as follow:

  1. Fit the regression with all the independent variables in the model.
  2. Calculate partial F-test for every variable in the model.
  3. Let F_L be the lowest of the partial F's. If the p-value for $F_L > \alpha_{stay}$ then remove the corresponding variable for the model and return to step 2 with one less variable. If p-value for $F_L \leq \alpha_{stay}$ then adopt the current model and no more variables are removed. The default in SAS is $\alpha_{stay} = 0.10$.

- Forward Selection: Start with no variables in the model. Add variables one-by-one until none meet the criteria for entry.

  1. Start with no variables in the model.
  2. Examine all variables not in the model and choose the one with the largest partial correlation. Calculate the partial F for the variable and label it F_U.

3. If the p-value for $F_U < \alpha_{entry}$ then add the corresponding variable to the model. Go to step 2. If the p-value for $F_U \geq \alpha_{entry}$ then do not add this or any other variable. Stop here. In SAS, the default for $\alpha_{entry} = 0.5$.

Forward selection is not very popular. Useful for explaining stepwise selection. Something important can be left out of the model due to overlap of information.

- Stepwise Regression: Stepwise regression is a blend of forward and backward selection. It begins with forward selection by adding variables one at a time. But, after a variable is entered, all others in the model are then tested to see if any can be thrown out. Once this is done, those not in the model are examined for entry, etc, etc... This procedure requires two significant levels: α_{entry} and α_{stay}. The defaults in SAS are $\alpha_{entry} = \alpha stay = 0.15$. Always keep $\alpha_{stay} \geq \alpha_{entry}$. Otherwise, variables added will be immediately removed.

SAS Code

```
CHOOSING A MODEL FOR THE HOSPITAL DATA. THIS EXAMPLE WILL DEMONSTRATE
IMPLEMENTATION OF THE VARIOUS VARIABLE SELECTION TECHNIQUES IN SAS;

OPTION NODATE;

DATA HOSPITAL;
INPUT X1-X5 Y;
IF (X1 > 199) THEN DELETE;
LABEL X1 = 'AVERAGE DAILY PATIENT LOAD'
X2 = 'MONTHLY X-RAY EXPOSURES'
X3 = 'MONTHLY OCCUPIED BED DAYS'
X4 = 'ELIGIBLE POP IN AREA(DIVIDED BY 1000)'
X5 = 'MONTHLY LABOR HOURS';
CARDS;
15.57 2463 479.92 18.0 4.45 566.52
...
510.22 86533 15524.00 371.6 6.35 18854.45
;

PROC REG DATA=HOSPITAL;
MODEL Y=X1-X5/SELECTION = FORWARD;
TITLE 'HOSPITAL DATA: FORWARD SELECTION';
RUN;


PROC REG DATA=HOSPITAL;
MODEL Y=X1-X5/SELECTION = BACKWARD;
TITLE 'HOSPITAL DATA: BACKWARD SELECTION';
RUN;


PROC REG DATA=HOSPITAL;
MODEL Y=X1-X5/SELECTION = STEPWISE INCLUDE=1 SLE=.10 SLS=.20;
TITLE 'HOSPITAL DATA: STEPWISE SELECTION';
RUN;


PROC REG DATA=HOSPITAL;
MODEL Y=X1-X5/SELECTION = RSQUARE CP MSE ADJRSQ BEST=10 STOP=5;
```

```
TITLE 'HOSPITAL DATA: RSQUARE SELECTION';
RUN;
```

Some of the options used are as follow: INCLUDE=1 means include the first variable in the model automatically, SLE=.10 is α_{entry}, SLS=.20 is α_{stay}, BEST=10 means only show the best 10 models with highest R^2, and STOP=5 means don't show any models with more than five variables in it.

11.11.3 Transforming X and Y to Get a Linear Fit

Polynomials are by no means the only families of models available to the regression worker. Here are some others: $y = \beta_0 + \beta_1 \left(\frac{1}{x_1}\right) + \beta_2 \left(\frac{1}{x_2}\right) + \epsilon$, $y = \beta_0 + \beta_1 \ln x_1 + \beta_2 \ln x_2 + \epsilon$, $y = \beta_0 + \beta_1 \sqrt{x_1} + \beta_2 \sqrt{x_2} + \epsilon$, or $\ln y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \epsilon$.

SAS Code

```
ANALYSIS USING A 2ND-ORDER RESPONSE SURFACE. THIS EXAMPLE IS ADAPTED
FROM NASA TECHNICAL MEMO 81556(1980): CYCLES TILL FAILURE OF
SILVER-ZINC CELLS WITH COMPETING FAILURE MODES-PRELIMINARY DATA
ANALYSIS. RESEARCHERS STUDIED THE EFFECT OF CHARGE RATE AND TEMPERATURE
ON A NEW TYPE OF POWER CELL. THE VARIABLES WERE
X1: CHARGE RATE(.6, 1.0, AND 1.4 AMPERES)
X2: TEMPERATURE(10, 20, 30C)
Y:  LIFE OF CELL MEASURED IN TERMS OF THE NUMBER OF DISCHARGE-CHARGE
    CYCLES BEFORE FAILURE.
NOT KNOWING THE NATURE OF THE RESPONSE FUNCTION, WE START WITH THE FULL
2-ND ORDER MODEL WHICH SEEMS TO OVERFIT THE DATA. NEXT STEP IS TO
DECIDE HOW TO PARE DOWN THAT MODEL. THE TEST STATEMENT IS ALSO
DEMONSTRATED;

DATA POWER;
INPUT X1 X2 Y;
X1SQ=X1**2; X2SQ=X2**2; X12=X1*X2;
CARDS;
0.6 10 50
1.0 10 86
1.4 10 49
0.6 20 88
1.0 20 157
1.0 20 131
1.0 20 184
1.4 20 109
0.6 20 179
1.0 30 235
1.4 30 224
;

PROC REG DATA=POWER;
MODEL Y = X1 X2 X1SQ X2SQ X12/R INFLUENCE;
LINONLY: TEST X1SQ=0 X2SQ=0 X12=0;
TITLE 'POWER CELLS EXAMPLE';
RUN;

PROC REG DATA=POWER;
MODEL Y = X1 X2 X1SQ X2SQ /R INFLUENCE;
```

```
LINONLY: TEST X1SQ=0 X2SQ=0;
RUN;

PROC REG DATA=POWER;
MODEL Y = X1 X2 X1SQ  X12/R INFLUENCE;
LINONLY: TEST X1SQ=0 X12=0;
RUN;

PROC REG DATA=POWER;
MODEL Y = X1 X2 X1SQ /R INFLUENCE;
OUTPUT OUT=NEW1 R=RESID STUDENT=STUDRES;
RUN;

PROC PLOT DATA=NEW1;
PLOT RESID*X1 RESID*X2;
RUN;

PROC UNIVARIATE PLOT NORMAL;
VAR STUDRES;
RUN;
```

SAS Code

```
THIS EXAMPLE IS FROM BOWERMAN AND O'CONNELL(PAGES 640-643). THE STATE
DEPARTMENT OF TAXATION WISHES TO INVESTIGATE THE TIME TO COMPLETE FORM
ST 1040 AVG AND ITS RELATIONSHIP TO THE
FILER'S EXPERIENCE IN FILLING IT OUT. WE EXPECT TIME TO DECAY WITH
EXPERIENCE, AND EXPECT AN ASYMPTOTIC BEHAVIOR TOWARDS A LOWEST BOUND.
NINE PEOPLE FOR WHOM INCOME AVERAGING IS ADVANTAGEOUS ARE RANDOMLY
SELECTED. WE INVESTIGATE TWO POSSIBLE MODELS FOR THE RELATIONSHIP;

DATA COMPLETE;
INPUT Y X @@;
XINV=1/X; LNX=LOG(X);
LNY=LOG(Y);

CARDS;
80 1 47 8 37 4 28 16 89 1 58 2 20 12 19 5 33 3;

PROC PLOT;
PLOT Y*X;
RUN;

PROC REG;
MODEL Y=XINV/R INFLUENCE;
OUTPUT OUT=NEW1 P=PREDICTD R=RES STUDENT=STUDRES;
TITLE 'MODEL 1';
RUN;

PROC UNIVARIATE NORMAL PLOT;
VAR STUDRES;
RUN;

PROC PLOT;
```

```
PLOT Y*X='O' PREDICTD*X='*'/OVERLAY;
PLOT Y*XINV='O' PREDICTD*XINV='*'/OVERLAY;
RUN;

PROC REG DATA=COMPLETE;
MODEL LNY=LNX;
OUTPUT OUT=NEW2 P=PREDICTD R=RES STUDENT=STUDRES;
TITLE 'MODEL 2';
RUN;

PROC UNIVARIATE NORMAL PLOT;
VAR STUDRES;
RUN;

PROC PLOT;
PLOT LNY*X='O' PREDICTD*X='*'/OVERLAY;
PLOT LNY*LNX='O' PREDICTD*LNX='*'/OVERLAY;
RUN;
```

11.12 Homework and Answers

Text, Chapter 10, # 5.

Text, Chapter 11, # 1, 7, 18. In # 18, you can use all of the techniques learned so far in this class. You are limited, however, to obtaining a final model that has at least 22 degrees of freedom for error. I will summarize the models chosen and show them to the class when the assignment is returned.

10.5: It seems that model # 2 has more multicollinearity. The p-values for most of the variables are large, thus indicating non-significance. We know that the t-statistic is calculated with $t = \frac{b_j}{s\sqrt{c_{jj}}}$. If c_{jj} which is related to multicollinearity is large(indicating much overlap of data), then the t statistic will be small which will give the impression that a $\beta_j = 0$ and thus the independent variable is not important. All of the variance inflation factors for the second model are much greater than 10. Thus, we can see that multicollinearity is seriously influencing the least squares point estimates.

11.1: $\bar{R}^2$ is the adjusted R^2 for the number of independent variables. $\bar{R}^2 = \left(R^2 - \frac{k-1}{n-1}\right)\left(\frac{n-1}{n-k}\right)$, where n is the number of observations and $k = p + 1$. Then, $\bar{R}^2 = \left(0.8628 - \frac{5-1}{18-1}\right)\left(\frac{18-1}{18-5}\right) = 0.8206$.

(b): The model with the smallest MS(E) is the 4-th model. It is also the model with the highest R^2 value. Additionally, the prediction interval is smallest with model 4.

Just by looking at the p-values, it does appear that model 3 is best in the table. But we know that multicollinearity could be influencing the p-values in model 4, thus making the p-values insignificant.

11.7: The usual residuals were calculated by taking the difference of the observed dependent variable and the predicted dependent variable. $e_i = y_i - \widehat{y}_i$, where $\widehat{y}_i = 2585.52 + 1.2324x_{i3} - 530.933x_{i5}$ where x_3 is the monthly occupied beds and x_5 is the average length of a patients stay in days.

The press residuals were calculated with the following equation: $d_i = \frac{e_i}{1-h_{ii}}$, where $h_{ii} = \mathbf{x}_i'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_i$ and e_i is the usual residual. We know that $d_{15} = \frac{e_{15}}{1-h_{15}}$. Substituting in values $-1448.866 = \frac{-469.07}{1-h_{15}}$. Solve for h_{15} to get 0.6763.

11.13 Remedies for Non-Constant Error Variance

Non-constancy of variances comes chiefly in one of two ways:

1. Var(y) is a function of some independent variable of x.
2. Var(y) is a function of E(y).

Correspondingly, there are two chief avenues for remedy:

1. A weighted analysis: divide the model by a function of x.
2. Apply a transformation: to y, then fit the model for the transformed y.

11.13.1 Weighted Analysis

If the residuals plot of e_i versus x_{ij} shows a fan pattern, then the Var(y) is a function of x_{ij}. We might suspect $\text{Var}(y_i) = \sigma_i^2$, where $\sigma_i = x_{ij}^c \sigma$ for some constant c. Consider the transformed model,

$$\frac{y_i}{x_{ij}^c} = \beta_0 \left(\frac{1}{x_{ij}^c}\right) + \beta_1 \left(\frac{x_{i1}}{x_{ij}^c}\right) + \beta_2 \left(\frac{x_{i2}}{x_{ij}^c}\right) + \cdots + \beta_p \left(\frac{x_{ip}}{x_{ij}^c}\right) + \frac{\epsilon_i}{x_{ij}^c}.$$

Let $y_i^* = \frac{y_i}{x_{ij}^c}$ for the dependent variable in this transformed model. Then,

$$\frac{Var(y_i^*)}{x_{ij}^{2c}} = \frac{1}{x_{ij}^{2c}}\sigma_i = \frac{x_{ij}^{2c}\sigma^2}{x_{ij}^{2c}} = \sigma^2.$$

The transformed model does not have the unequal variances problem. This is called the *weighted analysis*. The weights here are $w_i = \frac{1}{x_{ij}^{2c}}$. In general, weights are proportional to the reciprocal of the variance. The weighted analysis multiplies the model by $\sqrt{w_i}$.

SAS Code

Results of estimation and prediction using the weighted analysis: our estimate of μ_0 and our prediction of y_0 are $\widehat{y}_0 = b_0 + b_1 x_{01} + b_2 x_{02} + \cdots + b_p x_{0p}$. Our confidence interval for μ_0 is $\widehat{y}_0 \pm t_{\alpha/2}(n-k)s\sqrt{\mathbf{X}_0'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_0}$. Our prediction interval for y_0 is $\widehat{y}_0 \pm t_{\alpha/2}(n-k)s\sqrt{\mathbf{X}_{0j}^{2c} + \mathbf{X}_0'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{x}_0}$. Then, $\sigma_0^2 = \sigma^2 x_{0j}^{2c}$.

```
OPTION NODATE; LINESIZE=72; PS=30;

IN A STUDY OF 27 INDUSTRIAL ESTABLISHMENTS OF VARYING SIZES, THE NUMBER
OF SUPERVISED WORKERS(X) AND THE NUMBER OF SUPERVISORS(Y) WERE
RECORDED. IT WAS DECIDED TO STUDY THE RELATIONSHIP BETWEEN THE TWO
VARIABLES, AND AS A START A SIMPLE LINEAR MODEL WAS POSTULATED.;
*CHATTERJEE AND PRICE, 1991;

DATA SUPER;
INPUT X Y;
LABEL X='NUMBER OF WORKERS' Y='NUMBER OF SUPERVISORS';
CARDS;
294 30
247 32
267 37
358 44
423 47
311 49
```

```
450 56
534 62
438 68
697 78
688 80
630 84
709 88
627 97
615 100
999 109
1022 114
1015 117
700 106
850 128
980 130
1025 160
1021 97
1200 180
1250 112
1500 210
1650 135
750 .
;

PROC REG;
MODEL Y=X/XPX I CLM CLI;
OUTPUT OUT=NEW R=RESID P=PRED;
TITLE 'ORDINARY LEAST SQUARES ANALYSIS';
RUN;


PROC UNIVARIATE PLOT NORMAL;
VAR RESID;
RUN;

PROC PLOT;
PLOT Y*X='O' PRED*X='*'/OVERLAY;
PLOT RESID*X='*'/VREF=0;
RUN;

* THERE ARE TWO WAYS OT GO ABOUT A WEIGHTED ANALYSIS IN SAS. THE FAR
EASIER WAY IS SHOWN HERE -- THE OTHER WAY IS SHOWN IN THE TEXT BOOK.
CREATE A VARIABLE IN YOUR DATASET WHICH CONTAINS THE WEIGHTS YOU WANT TO
USE. THEN JUST RUN PROC REG AS USUAL BUT SPECIFY THE WEIGHTING VARIABLE
IN A 'WEIGHT' STATEMENT. SAS THEN DOES EVERY THING FOR YOU. ONE CAUTION-
IF YOU OUTPUT THE RESIDUALS TO PLOT, YOU WILL HAVE TO WEIGHT THEM
YOURSELF(SEE BELOW).

THE ALTERNATIVE METHOD, SHOWN IN OUR TEXT, IS TO TRANSFORM ALL OF THE
VARIABLES YOURSELF, AND THEN RUN THE TRANSFORMED MODEL WITH PROC REG.
NOT ONLY IS THIS A LOT OF EXTRA WORK, BUT THE CONFIDENCE INTERVALS
PRODUCED BY CLM AND CLI WILL BE FOR WEIGHTED UNITS, NOT THE ORGININAL
UNITS. I DO NOT RECOMMEND THAT APPROACH! ;
```

```
DATA SUPER1;
SET SUPER;
XSQ = X**2; XSQINV=1/XSQ;

PROC REG DATA=SUPER1;
MODEL Y=X/XPX I CLM CLI R INFULENCE;
WEIGHT XSQINV;
OUTPUT OUT=NEW1 R=RESID1 P=PRED1;
TITLE 'WEIGHTED LEAST SQUARES ANALYSIS';
RUN;

DATA NEW1;
SET NEW1;
WTRESID=RESID1/X;

PROC UNIVARIATE PLOT NORMAL DATA=NEW1;
VAR WTRESID;
RUN;

PROC PLOT DATA=NEW1;
PLOT Y*X='O' PRED1*X='*'/OVERLAY;
PLOT WTRESID*X='*'/VREF=0;
RUN;
```

11.13.2 Transformations of Y to Stabilize Variance

1. Try fixing everything else first. This may fix the non-normality problem.
2. If all else fails, try a transformation on y. The more popular one is the Box-Cox family of transformations: $y \rightarrow \frac{y^{\lambda}-1}{\lambda}$ for some λ.

SAS Code

```
OPTION NODATE; LS=72; PS=30;

* THIS IS EXAMPLE 13.5(PP 656-660);

DATA TEL;
INFILE 'BOC TAB134 A';
INPUT HOUR NORDERS @@;
Y=SQRT(NORDERS);
HOURSQ = HOUR**2;
LABEL HOUR = 'HOUR OF BUSINESS DAY'
HOURSQ = 'SQUARE OF HOUR'
NORDERS = 'NUMBER OF ORDERS'
Y = 'SQUARE ROOT OF NUMBER OF ORDERS';

PROC SORT;
BY HOUR;
RUN;

PROC UNIVARIATE PLOT;
BY HOUR; VAR NORDERS;
OUTPUT OUT=NEW1 MEAN=HOURMEAN VAR=HOURVAR STD=HOURSTD;
TITLE 'THE UNTRANSFORMED DATA';
```

```
RUN;

PROC PRINT DATA=NEW1;
RUN;

PROC REG DATA=TEL;
MODEL NORDERS = HOUR HOURSQ;
OUTPUT OUT=NEW1A STUDENT=STUDRES;
RUN;

PROC UNIVARIATE NORMAL PLOT DATA=NEW1A;
VAR STUDRES;
RUN;

PROC UNIVARIATE PLOT DATA=TEL;
BY HOUR; VAR Y;
OUTPUT OUT=NEW2 MEAN=HOURMEAN VAR=HOURVAR STD=HOURSTD;
TITLE 'DATA WITH TRANSFORMATION ON NUMBER OF ORDERS;
RUN;

PROC PRINT DATA=NEW2;
RUN;

PROC REG DATA=TEL;
MODEL Y = HOUR HOURSQ;
OUTPUT OUT=NEW2A STUDENT=STUDRES;
RUN;

PROC UNIVARIATE NORMAL PLOT DATA=NEW2A;
VAR STUDRES;
RUN;
```

11.14 Dummy Variables(Indicators)

Usually the independent variables in a regression model cover some continuous range. But, this need not always be the case. Consider the following example.

Example: 13 turkeys are measured for x as the age in weeks and y as the weight in pounds. 4 turkeys are from Georgia, 4 turkeys are from Virginia and 5 turkeys are from Wisconsin. Let

$$z_1 = \begin{cases} 1 & \text{if turkey from GA} \\ 0 & \text{if not} \end{cases}$$

$$z_2 = \begin{cases} 1 & \text{if turkey from VA} \\ 0 & \text{if not} \end{cases}$$

If $z1 = z2 = 0$, then the turkey must be from WI. In general, to represent a categorical variable with s levels, you need $s-1$ dummy variables. The model for turkeys is $y = \beta_0 + \beta_1 x + \beta_2 z_1 + \beta_3 z_2 + \epsilon$. The model for GA turkeys is $y = \beta_0 + \beta_1 x + \beta_2 + \epsilon = (\beta_0 + \beta_2) + \beta_1 x + \epsilon$. The model for VA turkeys is $y = (\beta_0 + \beta_3) + \beta_1 x + \epsilon$. The model for WI turkeys is $y = \beta_0 + \beta_1 x + \epsilon$. Can we get a model that does not assume the slope is the same for each state? Yes: $y = \beta_0 + \beta_1 x + z_1(\delta_0 + \delta_1 x) + z_2(\lambda_0 + \lambda_1 x) + \epsilon$. For WI turkeys: $y = \beta_0 + \beta_1 x + \epsilon$. For GA turkeys: $y = (\beta_0 + \delta_0) + (\beta_1 + \delta_1)x + \epsilon$. For VA turkeys: $y = (\beta_0 + \lambda_0) + (\beta_1 + \lambda_1)x + \epsilon$. These three models imply the following model: $y = \beta_0 + \beta_1 x_1 + \beta_2 z_1 + \beta_3 z_2 + \beta_4 z_1 x + \beta_5 z_2 x + \epsilon$. Let's test to see if VA turkeys and GA turkeys have the same model: $H_0 : \beta_2 = \beta_3$ or $H_0 : \beta_2 - \beta_3 = 0$. The general setup is $\mathbf{Y}$

$= \mathbf{X}\ \beta + \epsilon$. Let $\lambda' = (\lambda_0, \lambda_1, \lambda_2, \cdots, \lambda_p)$ be a vector of constants. Look at testing and estimation of $\lambda'\beta = \lambda_0\beta_0 + \lambda_1\beta_1 + \cdots + \lambda_p\beta_p$. For the turkey example:

$$\beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix}.$$

Here, $\lambda' = (0, 0, 1, -1)$. Here are the basic results:

1. The estimates of $\lambda'\beta$ are $\lambda'\mathbf{b}$.
2. The standard error of the estimate is $s_{\lambda'\mathbf{b}} = s\sqrt{\lambda'(\mathbf{X}'\mathbf{X})^{-1}\lambda}$.
3. The test statistic for $H_0 : \lambda'\beta = 0$ is $T = \frac{\lambda'\mathbf{X}}{s\sqrt{\lambda'(\ \mathbf{X}'\mathbf{X})^{-1}\lambda}}$. Reject H_0 if $|T| > t_{\alpha/2}(n-k)$.
4. A $(1-\alpha)100\%$ confidence interval for $\lambda'\beta$ is $\lambda'\mathbf{b} \pm t_{\alpha/2}(n-k)s\sqrt{\lambda'(\ \mathbf{X}'\mathbf{X})^{-1}\lambda}$.

SAS Code

```
USE OF INDICATOR VARIABLES. THIS EXAMPLE IS ON PAGE 243 OF DRAPER AND
SMITH. 13 TURKEYS HAVE BEEN MEASURED FOR THEIR HEIGHT, AGE AND STATE
OF ORIGIN;

DATA GOBBLER;
INPUT X Y  ORIGIN $ Z1 Z2;
Z1X = X1*X; Z2X = Z2*X;
LABEL X = 'AGE'
Y = 'WEIGHT'
ORGIN = 'STATE OF ORIGIN';

CARDS;
28 13.3 G 1 0
20 8.9 G 1 0
32 15.1 G 1 0
22 10.4 G 1 0
29 13.1 V 0 1
27 12.4 V 0 1
28 13.2 V 0 1
26 11.8 V 0 1
21 11.5 W 0 0
27 14.2 W 0 0
29 15.4 W 0 0
23 13.1 W 0 0
25 13.8 W 0 0
;

PROC REG;
MODEL Y = X Z1 Z2;
OUTPUT OUT=NEW P=PREDICTD;
NOSTATE: TEST Z1=0, Z2=0;
TITLE 'PARALLEL LINES MODEL';
RUN;

PROC PLOT;
```

```
PLOT Y*X=ORIGIN PREDICTD*X='*'/OVERLAY;
RUN;

PROC REG DATA=GOBBLER;
MODEL Y = X Z1 Z2 Z1X Z2X;
OUTPUT OUT=NEW1 P=PREDICTD;
SAMEINT: TEST Z1=0, Z2=0;
SAMESLOP: TEST Z1X=0, Z2X=0;
TITLE 'SEPARATE LINES(OR INTERACTION) MODEL';
RUN;

PROC PLOT;
PLOT Y*X=ORIGIN PREDICTD*X='*'/OVERLAY;
RUN;
```

11.14.1 Piece-wise Linear Regression

Another important use of dummy variables is for *piece-wise linear regression.*

```
|
|
|          b0 - b2x0 + (b1+b2)x
|       /-----------------------
|      /
|     /
|    /
|   /
|__________________________________________
```

We want a different slope to kick-in at $x = x_0$. The model is $y = \beta_0 + \beta_1 x + \beta_2(x - x_0)z + \epsilon$, where

$$z = \begin{cases} 1 & \text{if } x > x_0 \\ 0 & \text{if } x \leq x_0 \end{cases}$$

SAS Code

```
USE OF INDICATORS TO FIT A PIECEWISE LINEAR REGRESSION. THE DATA
FIRST APPEARED IN THE NEW YORK TIMES(SEPT 28, 1975). WE ARE TRYING
TO MODEL LIFE EXPECTANCY AS A FUNCTION OF PER-CAPITA INCOME;

OPTION NODATE;

DATA LIFEINC;
INPUT OBSNO COUNTRY $ LIFE INC;
LABEL COUNTRY = 'COUNTRY'
LIFE = 'LIFE EXPECTANCY'
INC = 'PER-CAPITA INCOME;
DROP OBSNO;

CARDS;
1 AUSTRALIA 71.0 3426
...
101 ZAIRE 38.8 118
;

PROC PLOT;
```

```
PLOT LIFE*INC;
RUN;

DATA LIFEINC1;
SET LIFEINC;
IF INC>1100 THEN Z1=1; ELSE Z1=0;
Z1INC=Z1*(INC-1100);
INCSQ=INC**2;

PROC REG;
MODEL LIFE=INC;
TITLE 'SIMPLE LINEAR REGRESSION';
RUN;

PROC REG;
MODEL LIFE=INC INCSQ;
TITLE 'QUADRATIC MODEL';
RUN;

PROC REG;
MODEL LIFE=INC Z1INC/R INFLUENCE;
OUTPUT OUT=NEW P=PREDICTD R=RESI STUDENT=STUDRESI COOKD=COOKS
   H=LEVERAGE DFFITS=DIFFITS;
ID COUNTRY;
TITLE 'PIECEWISE LINEAR MODEL';
RUN;

PROC PLOT;
PLOT LIFE*INC='O' PREDICTD*INC='*'/OVERLAY;
RUN;

PROC UNIVARIATE PLOT NORMAL;
VAR STUDRESI COOKS LEVERAGE;
ID COUNTRY;
RUN;
```

11.15 Homework and Answers

Text, Chapter 12, # 1,2,3,4(a,c),5(a,b,c,d,e),26,27,28.

12.1: $R^2 = 1 - \frac{SS(E)}{SS(TOTAL)} = 1 - \frac{45}{500} = 0.91$. 91% of the variation in the model is explained by the independent variables and the dummy variables.

$H_0: \beta_1 = \beta_2 = \beta_3 = \beta_4 = 0$ versus at least one $\beta \neq 0$. $F(MODEL) = \frac{MS(MODEL)}{MS(E)} = \frac{\frac{SS(MODEL)}{4}}{\frac{SS(E)}{25-5}} = \frac{\frac{500-45}{4}}{\frac{45}{20}} = \frac{113.75}{2.25} = 50.56$. $F_{0.05}(4,20) = 2.87$. Since $50.56 > 2.87$, reject H_0. At least one β does not equal zero.

12.2: $\mu_{[aC]} = \beta_0 + \beta_1 a + \beta_2 a^2 + \beta_3(0) + \beta_4(1)$, $\mu - [aA] = \beta_0 + \beta_1 a + \beta_2 a^2 + \beta_3(0) + \beta_4(0)$. $\mu_{[aC]} - \mu_{[aA]} = \beta_4$. $\mu_{[aB]} = \beta_0 + \beta_1 a + \beta_2 a^2 + \beta_3(1) + \beta_4(0)$. $\mu_{[aB]} - \mu_{[aA]} = \beta_3$. $\mu_{[aC]} - \mu_{[aB]} = \beta_4 - \beta_3$. $\beta_4 = \mu_{[aC]} - \mu_{[aA]}$ measures the effects on mean sales of video recorders when changing from advertiser A to advertiser C. $\beta_3 = \mu_{[aB]} - \mu_{[aA]}$ measures the effects on mean sales of video recorders when changing from advertiser A to advertiser B. $\beta_4 - \beta_3 = \mu_{[aC]} - \mu_{[aB]}$ measures the effects on mean sales of video recorders when changing from advertiser B to advertiser C.

12.3: $H_0 : \mu_{[aC]} = \mu_{[aB]} = \mu_{[aA]}$ versus at least one μ is not equal.
The complete model is $y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 D_{iB} + \beta_4 D_{iC}$. The reduced model is $y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \epsilon_i$. $F(D_{iB}, D_{iC} | x_{i1}, x_{i1}^2) = \frac{MS_{drop}}{MS(E)_{complete}} = \frac{\frac{SS_{drop}}{p-g}}{\frac{SS(E)_{comp}}{n-k}}$.

$$\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y} = \begin{pmatrix} 0.02 & 0 & 0 \\ 0 & 0.01 & 0 \\ 0 & 0 & 0.05 \end{pmatrix} \begin{pmatrix} 1000 \\ 300 \\ 50 \end{pmatrix} = \begin{pmatrix} 20 \\ 3 \\ 2.5 \end{pmatrix}.$$

For the reduced model,

$$SS(E)_{drop} = 21500 - \begin{pmatrix} 20 & 3 & 2.5 \end{pmatrix} \begin{pmatrix} 1000 \\ 300 \\ 50 \end{pmatrix} = 475.$$

For the complete model $SS(E)_{drop} = 475 - 45 = 430$. Then,

$$\frac{\frac{SS_{drop}}{4-2}}{\frac{SS(E)_{comp}}{25-5}} \frac{\frac{430}{2}}{\frac{45}{20}} = 95.56.$$

$F_{0.05}(2, 20) = 3.49$. Since $95.56 > 3.49$, reject H_0. At least 2 of the μ's are different or at least one $\beta \neq 0$. The partial F test says that the mean difference between agencies A and C and agencies A and B are significant and should not be removed from the model for at least one of them or both of them. In all practical sense, different advertising agencies do influence the mean sales of video recorders.

12.4: $H_0 : \beta_3 = 0$ versus $H_1 : \beta_3 \neq 0$. $t = \frac{b_3}{s\sqrt{c_{33}}} = \frac{3}{1.5\sqrt{0.05}} = 8.94$. $t_{0.025}(20) = 2.086$. Since $8.94 > 2.086$, reject H_0. $\beta_3 \neq 3$. There does exist a significant difference between advertising thru agency B and agency A. $b_3 \pm t_{0.025}(25)s\sqrt{c_{33}}$ $3 \pm 2.086(1.5)\sqrt{0.05}$ $(2.3, 3.7)$. This interval makes Panasound 95% confident that the effect of changing from agency A to agency B will increase sales between 2300 units and 3700 units.

12.5:

$$\lambda = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 1 \end{pmatrix}.$$

$$\begin{pmatrix} 0 & 0 & 0 & -1 & 1 \end{pmatrix} \begin{pmatrix} 0.02 & 0 & 0 & 0 & 0 \\ 0 & 0.01 & 0 & 0 & 0 \\ 0 & 0 & 0.05 & 0 & 0 \\ 0 & 0 & 0 & 0.05 & 0 \\ 0 & 0 & 0 & 0 & 0.10 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 1 \end{pmatrix} = 0.15.$$

$H_0 : \beta_4 - \beta_3 = 0$ versus $H_1 : \beta_4 - \beta_3 \neq 0$. $t = \frac{b_4 - b_3}{s\sqrt{\lambda'(\mathbf{X}'\mathbf{X})^{-1}\lambda}} = \frac{5-3}{1.5\sqrt{0.15}} = 3.44$. $t_{0.025}(2) = 2.086$. Since $3.44 > 2.086$, reject H_0. It can be concluded that the effects of advertising agencies B and C do differ.

12.27:

$$D_{iB} = \begin{cases} 1 & \text{if gas type B.} \\ 0 & \text{otherwise.} \end{cases}$$

$$D_{iC} = \begin{cases} 1 & \text{if gas type C.} \\ 0 & \text{otherwise.} \end{cases}$$

If $D_{iB} = D_{iC} = 0$, then the gas type is A.

The variable x_2(additive) plotted against y resembles an upside-down curve. We know that there is interaction between gas type and gas additive when plotted with the dependent variable. Thus, the two terms $D_{iB}x_{i2}$ and $D_{iC}x_{i2}$ should be in the model. The other three terms D_{iB}, D_{iC}, and x_{i2} are the usual independent variables that help predict gas mileage.

The y vector and the $\mathbf{X}$ matrix are

$$y = \begin{pmatrix} 28.0 \\ 28.6 \\ 27.4 \\ 33.3 \\ 34.5 \\ 33.0 \\ 32.0 \\ 35.6 \\ 34.4 \\ 35.0 \\ 34.0 \\ 33.3 \\ 34.7 \\ 33.5 \\ 32.3 \\ 33.4 \\ 33.0 \\ 32.0 \\ 29.6 \\ 30.6 \\ 28.6 \\ 29.8 \end{pmatrix}, X = \left(\begin{array}{ccccccccc} x_0 & D_{iB} & D_{iC} & x_2 & D_{ib}x_2 & D_{iC}x_2 & D_{iB}x_2^2 & D_{iC}x_2^2 & \\ \hline 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 2 & 4 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2 & 4 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 2 & 4 & 2 & 0 & 4 & 0 \\ 1 & 0 & 1 & 2 & 4 & 0 & 2 & 0 & 4 \\ 1 & 0 & 1 & 2 & 4 & 0 & 2 & 0 & 4 \\ 1 & 1 & 0 & 3 & 9 & 3 & 0 & 9 & 0 \\ 1 & 1 & 0 & 3 & 9 & 3 & 0 & 9 & 0 \\ 1 & 0 & 1 & 3 & 9 & 0 & 3 & 0 & 9 \\ 1 & 0 & 1 & 3 & 9 & 0 & 3 & 0 & 9 \end{array}\right).$$

12.28 $\mu_{Bx_2} = \beta_0 + \beta_1 + \beta_3 x_{i2} + \beta_4 x_{i2}^2 + \beta_5 x_{i2} + \beta_7 x_{i2}^2 + \epsilon_i$. $\mu_{Ax_2} = \beta_0 + \beta_3 x_{i2} + \beta_4 x_{i2}^2 + \epsilon_i$. $\mu_{Cx_2} = \beta_0 + \beta_2 + \beta_3 x_{i2} + \beta_4 x_{i2}^2 + \beta_6 x_{i2} + \beta_8 x_{i2}^2 + \epsilon_i$. $\mu_{Bx_2} - \mu_{Ax_2} = \beta_1 + \beta_5 x_{i2} + \beta_7 x_{i2}^2$. $\mu_{Cx_2} - \mu_{Ax_2} = \beta_2 + \beta_6 x_{i2} + \beta_8 x_{i2}^2$. $\mu_{Cx_2} - \mu_{Bx_2} = \beta_2 - \beta_1 + \beta_6 x_{i2} - \beta_5 x_{i2} + \beta_8 x_{i2}^2 - \beta_7 x_{i2}^2$. $\frac{\mu_{Cx_2} + \mu_{Bx_2}}{2} - \mu_{Ax_2} = \frac{\beta_1 + \beta_2 + \beta_5 x_{i2} + \beta_6 x_{i2} + \beta_7 x_{i2}^2 + \beta_8 x_{i2}^2}{2}$.

$\mu_{Bx_2} - \mu_{Ax_2}$ measures the effects on gas mileage when changing from unleaded gas type A to type B at a given amount of x_2. $\mu_{Cx_2} - \mu_{Ax_2}$ measures the effects on gas mileage when changing from unleaded gas type A to type C at a given amount of x_2. $\mu_{Cx_2} - \mu_{Bx_2}$ measures the effect on gas mileage when changing from unleaded gas type B to type C at a given amount of x_2. $\frac{\mu_{Cx_2} - \mu_{Bx_2}}{2} - \mu_{Ax_2}$ measures the effect on gas mileage when changing from unleaded gas type A to the average of C and B.

11.16 1-Factor Experiments

One version of the model statement is $y_{lk} = \mu_l + \epsilon_{lk}$, where μ_l is the average response at the l-th level, and ϵ_{lk} is the error. The usual assumptions for ϵ_{lk} are normality, independence and constancy. Alternate way of writing the model is $y_{lk} = \mu + \tau_l + \epsilon_{lk}$. If a 1-factor model has v numeric variables, then it is equivalent to a $v - 1$ degree polynomial model.

In the caffeine example in the SAS Code section, $v = 3$. There are 3 levels of caffeine. The first test is $H_0 : \mu_1 = \mu_2 = \mu_3$, versus H_1 : at least one mean is not equal. If we reject the overall test, we need to look closely at where the differences are. There are two techniques:

1. Multiple comparisons: test all pairs $\mu_l - \mu_{l'}$, which controls use of one which has the smallest coefficient.

2. Estimate and test the more general linear function $\sum_{l=1}^{v} c_l \mu_l$, where $\sum c_l = 0$. These are called *contrasts*. The estimation of a contrast is $\sum_{l=1}^{v} c_l \bar{y}_l$, where $\bar{y}_l$ is the sample mean at level l. The *standard error* is $s\sqrt{\sum_{l=1}^{v} \frac{c_l^2}{n_l}}$. Hence the confidence interval is $\sum_{l=1}^{v} c_l \bar{y}_l \pm t_{\alpha/2}(\sum n_l - v) s \sqrt{\sum_{l=1}^{v} \frac{c_l^2}{n_l}}$. The test statistic is $t = \frac{\sum c_l \mu_l}{s\sqrt{\sum \frac{c_l^2}{n_l}}}$ Reject H_0 if $|t| > t_{\alpha/2}(\sum n_l - v)$.

SAS Code

```
*THREE DIFFERENT RUNS OF THE SAME 1-WAY ANOVA DATA;
*SEE HANDOUT FOR AN EXPLANATION OF THE EXPERIMENT THAT
PRODUCED THESE DATA;

OPTIONS NODATE;

DATA TABLE9_1;
INPUT CAFFEINE TAPS @@;
IF CAFFEINE=1 THEN D1=1; ELSE D1=0; *D1 AND D2 ARE ONE POSSIBLE SET;
IF CAFFEINE=2 THEN D2=1; ELSE D2=0; * OF INDICATOR VARIABLES;
CAFFSQ=CAFFEINE**2; *CAFFSQ WILL BE USED IN A QUADRATIC REG;
CARDS;
1 242 1 245 1 244 1 248 1 247 1 248 1 242 1 244 1 246 1 242
...
;

PROC PRINT;
TITLE 'THE DATA AND THE INDICATOR VARIABLES';
RUN;

PROC SORT; BY CAFFEINE;
PROC UNIVARIATE PLOT;
VAR TAPS; BY CAFFEINE;
TITLE 'VISUAL DISPLAY SHOWING EACH LEVEL OF THE EXPERIMENTAL VALUE';
RUN;

PROC REG;
MODEL TAPS = D1 D2;
TITLE 'ONE-WAY ANOVA WITH INDICATORS Z1 AND Z2';

PROC REG;
MODEL TAPS = CAFFEINE CAFFSQ/SS1 SS2;
TITLE 'THE QUADRATIC REGRESSION MODEL';
RUN;

PROC GLM;
MODEL TAPS = CAFFEINE;
MEANS CAFFEINE/BON TUKEY SCHEFFE;
OUTPUT OUT=NEW R=RESI COOKD=COOKS;
TITLE 'THE ONE-WAY ANOVA USING GLM';
RUN;

PROC UNIVARIATE PLOT NORMAL;
VAR RESI;
TITLE 'RESIDUALS FOR ENTIRE DATA SET';
RUN;
```

SAS Code

```
*DEMONSTRATION OF THE CONTRAST STATEMENT IN PROC GLM;
*SHOWING THE SAME TESTS WITH THE REG REGRESSION;
* THIS IS THE SAME DATA AS IN THE PREVIOUS SECTION;
```

```
OPTIONS NODATE;

DATA TABLE9_1;
INPUT CAFFEINE TAPS @@;
IF CAFFEINE=1 THEN D1=1; ELSE D1=0; *D1 AND D2 ARE ONE POSSIBLE SET;
IF CAFFEINE=2 THEN D2=1; ELSE D2=0; * OF INDICATOR VARIABLES;
CARDS;
1 242 1 245 1 244 1 248 1 247 1 248 1 242 1 244 1 246 1 242
...
;

PROC GLM;
CLASS CAFFEINE;
MODEL TAPS = CAFFEINE;
MEANS CAFFEINE/LSD;
CONTRAST '0MG VS 200MG' CAFFEINE 1 0 -1;
CONTRAST '100MG VS AVG OF OTHERS' CAFFEINE 1 -2 1;
CONTRAST '100MG VS 200MG' CAFFEINE 0 -1 1;
TUTLE 'ANALYSIS OF COFFEE DATA';
RUN;

PROC REG;
MODEL TAPS = D1 D2;
CF0VS200: TEST D1=0;
AVGVS100: TEST D1-2*D2=0;
CF100200: TEST -D2=0;
RUN;
```

SAS Code

```
* ANOTHER 1-WAY ANOVA EXAMPLE. THE GROUPING VARIABLE IS
NON-NUMERIC, SO A POLYNOMIAL MODEL DOESN'T HAVE ANY
INTERPRETATION OR MAKE SENSE LIKE IN EXAMPLE 19. BUT THIS
DOESN'T KEEP US FROM DEFINING DUMMY VARIABLES THAT WILL
RUN THE ANOVA AS A REGRESSION, WHICH IS DONE IN THE PROC
REG BELOW. NEVERTHELESS, WE PREFER TO RUN THE ANOVA WITH
PROC GLM, WHICH IS SHOWN AFTER THE REG. THE GLM APPROACH
IS EASIER TO CODE AND THE RESULTS ARE EASIER TO INTERPRET.
THE REG APPROACH IS SOLELY TO HELP US UNDERSTAND THAT
ANALYSIS OF VARIANCE IS A SPECIAL CASE OF REGRESSION,
EVEN THOUGH WE DON'T USUALLY THINK OF IT IN THAT WAY;

* THIS EXAMPLE IS TAKEN FROM BOWERMAN & OCONNELL (PAGE 786).
TO COMPARE THE DURABILITY OF FOUR DIFFERENT BRANDS OF GOLF
BALLS, FIVE OF EACH BRAND ARE SELECTED AND PLACED INTO A
MACHINE THAT EXERTS THE FORCE OF A 250 YARD DRIVE. THE
NUMBER OF SIMULATED DRIVES NEEDED TO BREAK OR CHIP EACH
BALL IS RECORDED;

OPTION NODATE;

DATA HACKER;
INPUT BRAND $ DRIVES @ @;
IF BRAND='ALPHA' THEN Z1=1; ELSE Z1=0;
```

```
IF BRAND='BEST' THEN Z2=1; ELSE Z2=0;
IF BRAND='CENTURY' THEN Z3=1; ELSE Z3=0;
CARDS;
ALPHA 281 ALPHA 220 ALPHA 274 ALPHA 242 ALPHA 251
...
;

PROC SORT; BY BRAND;
RUN;

PROC UNIVARIATE PLOT;
VAR DRIVES;
BY BRAND;
TITLE 'VISUAL DISPLAY OF DATA ON EACH BRAND';
RUN;

PROC REG;
MODEL DRIVES= Z1 Z2 Z3;
CONTRAST1: TEST Z1+Z2+Z3=0;
CONTRAST2: TEST Z1-Z2+Z3=0;
TITLE 'ONE-WAY ANOVA WITH INDICATORS';
RUN;

PROC GLM;
CLASS BRAND;
MODEL DRIVES=BRANDS;
MEANS BRAND/LSD;
CONTRAST 'DIVOT VS OTHERS' BRAND -1 -1 -1 3;
CONTRAST 'ALPHA/CENT VS BEST/DIV' BRAND 1 -1 1 -1;
ESTIMATE 'ALPHA/CENT VS BEST/DIV' BRAND 1 -1 1 -1;
ESTIMATE 'DIVOT MEAN' INTERCEPT 1 BRAND 0 0 0 1;
OUTPUT OUT=NEW R=RESI COOKD=COOKS;
TITLE 'THE ONE-WAY ANOVA USING PROC GLM';
RUN;

PROC SORT; BY BRAND;
RUN;

PROC UNIVARIATE PLOT NORMAL;
VAR RESI;
TITLE 'RESIDUALS FOR ENTIRE DATA SET';
RUN;

PROC UNIVARIATE PLOT;
VAR COOKS;
TITLE 'COOK'S D FOR ENTIRE DATA SET';
RUN;
```

11.17 2-Factor Experiments

In a 2-factor experiment, we have two factors to be assessed for their effects on a response variable. The model is $y_{ijk} = \mu_{ij} + \epsilon_{ijk}$, where y_{ijk} is the k-th response using level i of factor 1 and with level j of factor 2. μ_{ij} is the mean response when using the combination of level i of factor 1 and level j of factor

2. ϵ_{ijk} is the error with the usuall assumptions. An alternative way of writing the model statement is $y_{ijk} = \mu + \alpha_i + \gamma_j + \theta_{ij} + \epsilon_{ijk}$, where μ is the overall mean, α_i is the effect of level i of factor 1, γ_j is the effect of level j of factor 2, θ_{ij} is the interaction of the i-th level of factor 1 with the j-th level of factor 2.

The primary questions are:

1. Do the factors interact?
2. How does changing the level of factor 1 affect the response?
3. How does changing the level of factor 2 affect the response?

Consider the example in the text book: consider changing from level 1 to leve 2 of shelf height. If width is equal to regular, the response is $\mu_{21} - \mu_{11} = (\mu + \alpha_2 + \gamma_1 + \theta_{21}) - (\mu + \alpha_1 + \gamma_1 + \theta_{11}) = (\alpha_2 - \alpha_1) + (\theta_{21} + \theta_{11})$. If the width is wide, then the change in response is $\mu_{22} - \mu_{12} = (\mu + \alpha_2 + \gamma_2 + \theta_{22}) - (\mu + \alpha_1 + \gamma_2 + \theta_{12}) = (\alpha_2 - \alpha_1) + (\theta_{22} - \theta_{12})$. If no interaction, then the answer is the same whether we look at wide or regular shelves. But, if the factors interact, the answer for wide shelves is different than that for regular shelves.

SAS Code

```
* EXAMPLE OF A 2-FACTOR EXPERIMENT. DEMAND FOR A PRODUCT IS STUDIED AS
A FUNCTION OF SHELF DISPLAY HEIGHT(AT THREE LEVELS: BOTTOM, MIDDLE,
AND TOP) AND DISPLAY WIDTH(AT TWO LEVELS: REGULAR AND WIDE). THREE
MEASUREMENTS HAVE BEEN OBTAINED AT EACH FACTOR COMBINATION. THIS DATA
FORMS THE MAIN EXAMPLE IN CHAPTER 15 OF OUR TEXT;

OPTION NODATE LS=72 PS=40;

DATA SALES;
INPUT A B Y @@;
IF A=1 THEN DA1=1; ELSE DA1=0;
IF A=2 THEN DA2=1; ELSE DA2=0;
IF B=1 THEN DB1=1; ELSE DB1=0;
DAB11=DA1*DB1; DAB21=DA2*DB1;
LABEL A = 'DISPLAY HEIGHT'
B = 'DISPLAY WIDTH'
Y = 'MONTHLY DEMAND';
CARDS;
1 1 58.2 1 1 53.7 1 1 55.8
...
;

PROC FORMAT;
VALUE DW 1='BOTTOM' 2='MIDDLE' 2='TOP';
VALUE DH 1='REGULAR' 2='WIDE';
RUN;

* LET'S FIRST MAKE A MEANS PLOT FOR THE SIX COMBINATIONS - THIS IS
AN IMPORTANT GRAPHICAL TOOL IN ANALYZING TWO-FACTOR EXPERIMENTS;

PROC MEANS NOPRINT DATA=SALES;
CLASS A B;
VAR Y;
OUTPUT OUT=MEANDAT MEAN=SALESAVG;
RUN;
```

```
PROC PRINT DATA=MEANDAT;
RUN;

DATA MEANDAT;
SET MEANDAT; IF (_N_>6.5);

PROC PLOT DATA=MEANDAT;
FORMAT A DW. B DH.;
PLOT SALESAVG*A=B;
PLOT SALESAVG*B=A;
TITLE 'MEANS PLOTS FOR SHELF DATA';
RUN;

PROC REG DATA=SALES;
MODEL Y=DA1 DA2 DB1 DAB11 DAB21;;
HITETEST: TEST DA1+.5*DB1+.5DAB11-DA2-.5DB1-.5DAB21=0,
         DA2+.5DB1+.5DAB21-.5DB1=0;
WIDTEST: TEST 3*DB1+DAB11+DAB21=0;
INTTEST: TEST DAB11=0, DAB21=0;
TITLE1 'SHELF DISPLAY DATA';
TITLE2 'THE REGRESSION APPROACH';

* THE TESTS SHOWN IN PROC REG ARE THE STANDARD TESTS FOR A 2-FACTOR
ANOVA. THEY ARE A BIT MESSY TO WRITE IN TERMS OF THE INDICATORS. ONE
ADVANTAGE OF THE ANOVA APPROACH WITH PROC GLM IS THAT THESE TESTS
ARE GENERATED AUTOMATICALLY FOR YOU;

PROC GLM DATA=SALES;
FORMAT A DW. B DH.;
CLASS A B;
MODEL Y=A B A*B;
OUTPUT OUT=NEW2 R=RESI COOKD=COOKS;
TITLE2 'THE ANOVA APPROACH';
RUN;

PROC UNIVARIATE PLOT NORMAL;
VAR RESI COOKS;
TITLE 'RESIDUAL ANALYSIS';
RUN;

* SINCE THE INTERACTION TERM IS HIGHLY INSIGNIFICANT, WE MAY WANT TO
REMOVE IT FROM THE MODEL. THIS WILL RESULT IN MORE D.F. FOR THE
ERROR TERM, AND IS USUALLY CALLED POOLING THE INTERACTION WITH ERROR.
WITH THE INTERACTION TERM REMOVED FROM THE MODEL, WE EFFECTIVELY
ANALYZE EACH FACTOR AS IF THE OTHER WAS NOT PRESENT;


PROC GLM DATA=SALES;
FORMAT A DW. B DH.;
CLASS A B;
MODEL Y=A B;
CONTRAST 'TOP VS OTHERS' A -1 -1 2;
ESTIMATE 'WIDE SHELF MEAN' INTERCEPT 1 B 0 1;
MEANS A B / TUKEY BON;
```

```
MEANS A / TUKEY BON CLDIFF; * THIS OPTION EXPRESSES THE COMPARISONS IN
TERMS OF CONFIDENCE INTERVALS;
TITLE 'SHELF DISPLAY DATA WITH INTERACTION TERM POOLED TO ERROR';
RUN;

* ONE CONTRAST STATEMENT AND ONE ESTIMATE STATEMENT HAVE BEEN SHOWN
AS EXAMPLES - MANY OTHERS COULD BE DONE. SINCE THERE IS NO INTERACTION
IN THE MODEL, TESTS AND CONFIDENCE INTERVALS INVOLVING LEVELS OF A DO
NOT INVOLVE LEVELS OF B, AND VICE-VERSA;
```

SAS Code

```
* ANOTHER EXAMPLE OF A 2-WAY CROSS-CLASSIFICATION. THIS DATA, FROM THE
JOURNAL OF QUALITY TECHNOLOGY(1969) VIA DRAPER AND SMITH(1981),
CONCERNS A PROBLEM WITH PRODUCTION RATES IN A CATALYST PLANT. AFTER
EXTENSIVE DISCUSSION IN THE RESEARCH UNIT, IT WAS DECIDED TO FOCUS
THE INVESTIGATION ON FOUR REAGENTS AND THREE CATALYSTS;

OPTION NODATE; LS=72 PS=40;

DATA JQT;
INPUT REAGENT $ CATALYST PRODRATE @@;
IF REAGENT='A' THEN Z1=1; ELSE Z1=0;
IF REAGENT='B' THEN Z2=1; ELSE Z2=0;
IF REAGENT='C' THEN Z3=1; ELSE Z3=0;
IF CATALYST=1 THEN W1=1; ELSE W1=0;
IF CATALYST=2 THEN W2=1; ELSE W2=0;
ZW11=Z1*W1; ZW12=Z1*W2;
ZW21=Z2*W1; ZW22=X2*W2;
ZW31=Z3*W1; ZW32=Z3*W2;
CARDS;
A 1 4 A 1 6 A 2 11 A 2 7 A 3 5 A 3 9
...
;

* FIRST, THE MEANS PLOT;

PROC MEANS NOPRINT;
CLASS REAGENT CATALYST;
VAR PRODRATE;
OUTPUT OUT=MEANDAT MEAN=PRATEAVG;
RUN;

DATA MEANDAT;
SET MEANDAT; IF (_N_>8.5);


PROC PLOT DATA=MEANDAT;
PLOT PRATEAVG*REAGENT=CATALYST;
PLOT PRATEAVG*CATALYST=REAGENT;
TITLE 'MEANS PLOTS FOR PRODUCTION DATA';
RUN;

PROC REG DATA=JQT;
```

```
MODEL PRODRATE = Z1 Z2 Z3 W1 W2 ZW11 ZW12 ZW21 ZW22 ZW31 ZW32;
REAT: TEST 3*Z1+ZW11+ZW12, 3*Z2-3*Z1+ZW21+ZW22-ZW11-ZW12,
   3*Z3-3*Z2+ZW31+ZW32-ZW21-ZW22;
INTERACT: TEST ZW11, ZW12, ZW21, ZW22, ZW31, ZW32;
TITLE 'THE REGRESSION APPROACH';
RUN;

PROC GLM DATA=JQT;
CLASS CATALYST REAGENT;
MODEL PRODRATE=REAGENT CATALYST REAGENT*CATALYST;
TITLE 'THE ANOVA APPROACH';
RUN;

* SINCE THE INTERACTION IS PLAYING A STRONG ROLE, ONE OPTION IS TO
EXAMINE THE 4*3=12 TREATMENT COMBINATIONS AS LEVELS OF A SINGLE
FACTOR, WHICH CAN BE DONE WITH A 1-FACTOR ANOVA;

DATA NEW;
SET JQT;
IF REAGENT='A' THEN DO;
IF CATALYST=1 THEN TREAT='A1';
ELSE IF CATALYST=2 THEN TREAT='A2';
ELSE TREAT='A3';
END;

IF REAGENT='B' THEN DO;
IF CATALYST=1 THEN TREAT='B1';
ELSE IF CATALYST=2 THEN TREAT='B2';
ELSE TREAT='B3';
END;

IF REAGENT='C' THEN DO;
IF CATALYST=1 THEN TREAT='C1';
ELSE IF CATALYST=2 THEN TREAT='C2';
ELSE TREAT='C3';
END;

IF REAGENT='D' THEN DO;
IF CATALYST=1 THEN TREAT='D1';
ELSE IF CATALYST=2 THEN TREAT='D2';
ELSE TREAT='D3';
END;

KEEP PRODRATE TREAT;

PROC PRINT;
RUN;

PROC GLM DATA=NEW;
CLASS TREAT;
MODEL PRODRATE=TREAT;
MEANS TREAT/TUKEY BON;
OUTPUT OUT=NEW1 R=RESI COOKD=COOKS;
TITLE 'ANALYZING DATA AS 1-WAY CLASSIFICATION DUE TO INTERACTION';
```

```
RUN;

PROC UNIVARIATE PLOT NORMAL;
VAR RESI COOKS;
TITLE 'RESIDUAL ANALYSIS';
RUN;
```

11.18 Homework and Answers

1. We were asked to solve Problem 14.46 in the text book. We were asked to analyze the data using `PROC GLM` and `PROC REG` for a 1-factor experiment. In addition, we were asked to run an overall test to see if there are any differences in the factor levels, to use a multiple comparisons technique to investigate any differences in the factor levels, to calculate a few contrasts in means, and finally to verify the assumptions of the model.

   We are to predict aptitude test scores based on 5 levels of college degree type. The 5 levels are: Business, Science, Liberal Arts, Fine Arts, and Engineering. The 5 levels can be represented with the following dummy variables:

$$D1 = \begin{cases} 1, & \text{if degree type is Business} \\ 0, & \text{if degree type is not Business} \end{cases}$$

$$D2 = \begin{cases} 1, & \text{if degree type is Science} \\ 0, & \text{if degree type is not Science} \end{cases}$$

$$D3 = \begin{cases} 1, & \text{if degree type is Liberal Arts} \\ 0, & \text{if degree type is not Liberal Arts} \end{cases}$$

$$D4 = \begin{cases} 1, & \text{if degree type is Fine Arts} \\ 0, & \text{if degree type is not Fine Arts} \end{cases}$$

$$D5 = \begin{cases} 1, & \text{if not Business, Science, Liberal Arts, or Fine Arts} \\ 0, & \text{otherwise} \end{cases}$$

   Note that it only takes 4 dummy variables to model the 5 independent variables. This is because if `D1, D2, D3,` and `D4` are all equal to zero, then it can be deduced that the degree type is Engineering.

   The model statement produced by `PROC REG` appears as follow: $TESTS = 80.6 - 27.88D1 - 5.63D2 - 27D3 - 40.13D4$. Both `PROC REG` and `PROC GLM` produced similar results.

   Approximately 72% of the variation in the model can be explained by the 5 levels of college degree type(or 4 dummy variables). It appears that `D2` (Science) does not contribute much information to the model. This could be that there is overlapping information with the Engineering variable. We could look at the variance inflation factor to determine whether or not this is the case. But, we were not asked to do this. The overall F-test that tested whether any of the coefficients were not equal to zero had a p-value of 0.0001. Thus we reject the null hypothesis that all of the coefficients are equal to zero. We can conclude that one or more are not equal to zero. A multiple comparisons test was run to determine which factor levels differed from each other. The results using Tukey's method shows that there is a significant difference between both Engineering and Science test scores together, and Liberal Arts, Business and Fine Arts test scores together. That is to mean that there is no significant difference between Engineering and Science test scores, and that there is no significant difference among Liberal Arts, Business, and Fine Arts test scores.

Further tests were made concerning the differences in means. The means of each dummy variable are as follow: $\mu_{D1} = \beta_0 + \beta_1 D_1$. $\mu_{D2} = \beta_0 + \beta_2 D_2$. $\mu_{D3} = \beta_0 + \beta_3 D3$. $\mu_{D4} = \beta_0 + \beta_4 D4$. $\mu_{D5} = \beta_0$. Even though `D5` for Engineering is not explicitly stated in the model, it is implied to be the y intercept. The following is a list of specific tests performed:

(a) We tested for the difference in average test scores for Science and Engineering. This can be written as: $\mu_{D2} - \mu_{D5} = \beta_0 + \beta_2 D2 - \beta_0 = \beta_2 D2 = 0$. The result of this test shows that there is no significant difference in average test scores for Science and Engineering students at the 95% confidence level. This is the same result obtained by Tukey's method.

(b) We tested for the difference between business and the average of the two arts majors. This can be written as:

$$\mu_{D1} - \frac{\mu_{D3} + \mu_{D4}}{2} = \beta_0 + \beta_1 D1 - \frac{1}{2}\beta_0 - \frac{1}{2}\beta_3 D3 - \frac{1}{2}\beta_0 - \frac{1}{2}\beta_4 D4 =$$

$$\beta_1 D1 - \frac{1}{2}\beta_3 D3 - \frac{1}{2}\beta_4 D4 = 0.$$

The result of this test shows that there is no significant difference in average test scores for the difference between Business majors and the average of the two arts majors at the 95% confidence level.

(c) We tested for the difference between the average of Science and Engineering majors and the average of the other three majors. This can be written as:

$$\frac{\mu_{D2} + \mu_{D5}}{2} - \frac{\mu_{D1} + \mu_{D3} + \mu_{D4}}{3} = \frac{\beta_0 + \beta_2 D2 + \beta_0}{2} - \frac{\beta_0 + \beta_1 D1 + \beta_0 + \beta_3 D3 + \beta_0 + \beta_4 D4}{3} =$$

$$\frac{1}{2}\beta_2 D2 - \frac{1}{3}\beta_1 D1 - \frac{1}{3}\beta_3 D3 - \frac{1}{3}\beta_4 D4 = 0.$$

The result of this test shows that there is a significant difference between the average of Science and Engineering majors and the average of the other three majors at the 95% confidence level.

Finally, the assumptions of the model were verified using plots. The residuals were plotted against each of the independent variables. The results show a random pattern for all the variables. Thus constant variance holds true. A stem-and-leaf plot was used to verify the Normality assumption. The residuals appear to be Normally distributed. Thus the assumptions of the model have not been violated.

2. In problem 15.6, we were asked to model the effects of time of day and positioning of advertisements on tele-marketing response. This is a two factored experiment where Factor 1 is the time of day and Factor 2 is positioning of advertisements. Factor 1 has 3 levels: 10:00 morning (rerun of the Honeymooners), 4:00 afternoon(rerun of MASH), and 9:00 evening(first run of Cheers). Factor 2 has 4 levels: on the hour, on the half-hour, early in the program, and late in the program. We were to model this experiment using `PROC GLM`.

The first thing we needed to determine was whether or not interaction between the two factors were significant. That is because our interpretation of the model would be different if interaction is significant. As it turns out, in this experiment interaction is not significant. This was demonstrated in two ways: 1) the p-value for the mean response of interaction was very large, and 2) the plots of the means vs each independent variable showed parallel patterns. The interaction term was removed from the model and `PROC GLM` was run again.

Both means of the independent variables appear to be significant. 99% of the variation is explained by the model. Using Tukey's method to determine which levels of the two factors differed, it was determined that for the positioning of advertisements, early in the program differed significantly from late in the program, from on the hour and from on the half-hour. Late in the program differed significantly from on the hour and on the half-hour. However, on the hour and on the half-hour did not differ significantly from each other. Again using Tukey's method on the time of tele-marketing, all three levels differed significantly from each other. That is to say that the mean response of 9:00 evening, 4:00 afternoon, and 10:00 morning differed significantly at the 95% level.

`PROC UNIVARIATE` was run on Cook's D statistic. It showed that observation 20 may be an outlier.

To test the constant variance assumption, plots of the residuals and factors were made. Both plots(one for each factor) showed random patterns. Thus, constance variance does hold true. `PROC UNIVARIATE` was run on the residuals. A Normally distributed pattern appeared in the stem and leaf diagram. Thus, the Normality assumption holds true.

11.19 Logistic Regression

The reference book used in this section is *Applied Logistic Regression,* Homser and Lemeshow, Wiley(1989).

Logistic regression is regression with a binary response variable. An example would be letting y be the presence of coronary heart disease and the independent variables being age, cholesterol, weight, etc. In general, logistic regression deals with regression models for binary response variables. The independent variables can be continuous, categorical, or both as usual. The distinguishing characteristic is that y has only 2 values and thus is not normal. Note that direct prediction of y is useless. Since y can only be 0 or 1, and both are possible at any x, what we will do is model, like in ordinary regression, the expected value of y. $E(y|x) = P(y=1|x)1 + P(y=0|x)0 = P(y=1|x) = \Pi(x)$, which is the probability of having a coronary disease in the example. The models we will use are *intrinsically linear:* as stated, they do not appear to be linear, but become so with a suitable transformation. NOTE: Invert 0 and 1, you would get the model for people without heart disease. The *logistic model* fits s-shaped curves. s-shaped curves

$$\Pi(x) = \frac{e^{\beta_0+\beta_1 x}}{1+e^{\beta_0+\beta_1 x}}.$$

This can be transformed to a linear model as follow:

$$1-\Pi(x) = \frac{1}{e^{\beta_0+\beta_1 x}} \Rightarrow \frac{\Pi(x)}{1-\Pi(x)} = e^{\beta_0+\beta_1 x} \Rightarrow \ln\left(\frac{\Pi(x)}{1-\Pi(x)}\right) = \beta_0+\beta_1 x.$$

How about the error terms? With $\Pi(x)$, as given above, the model is $y = \Pi(x) + \epsilon$. But, unlike in ordinary regression, ϵ is not normal, since y has only 2 possible values. $y = 1 \Rightarrow \epsilon = 1-\Pi(x)$, and $y = 0 \Rightarrow \epsilon = -\Pi(x)$,

11.19.1 Fitting the Logistic Regression Model

In ordinary regression, we fit the model $y_i = \beta_0 + \beta_1 x_i + \epsilon_i$ by least sum of squares. With the normal distribution, the joint density for $y_1, y_2, ..., y_n$ is

$$f(y_1, y_2, ..., y_n) = \frac{1}{(2\pi)^{n/2}} \frac{1}{\sigma^n} \exp\left(-\frac{1}{2}\sum_{i=1}^{n} \frac{(y_i-\beta_0-\beta_1 x_i)^2}{\sigma^2}\right)$$

which for purposes of estimation is called the *likelihood.* Maximizing the likelihood function is the same as minimizing SS(E). The technique is called *maximum likelihood estimation* say to estimate β_0 and β_1 by maximizing the likelihood function. In this course, we have presented regression as an estimation technique based on minimizing SS(E) — the underlying reason for doing that is that it *maximizes the likelihood.* Maximum likelihood is the fundamental principle of estimation, and is what we shall use for the logistic regression model.

For our simple logistic regression model, the parameters are $\beta = (\beta_0, \beta_1)$. The likelihood function is

$$L = \prod_{i=1}^{n} \Pi(x_i)^{y_i}[1-\Pi(x_i)]^{1-y_i}.$$

The *log likelihood* is

$$\log L = \sum_{i=1}^{n} \left(y_i \ln[\Pi(x_i)] + (1 - y_i) \ln[1 - \Pi(x_i)] \right).$$

We want to find the values b_0, and b_1 of β_0 and β_1 which maximizes L. So, evaluate $\frac{\partial L}{\partial \beta_0}$ and $\frac{\partial L}{\partial \beta_1}$, which yields

$$\sum_{i=1}^{n} (y_i - \Pi(x_i)) = 0$$

and

$$\sum_{i=1}^{n} x_i [y_i - \Pi(x_i)] = 0.$$

There is no explicit analytic solution to these equations. Solutions are found computationally by a computer algorithm. Note that a consequence of the first equation is

$$\sum_{i=1}^{n} \frac{y_i}{n} = \sum_{i=1}^{n} \frac{\widehat{\Pi}(x_i)}{n}.$$

SAS Code

```
* THE AGE AND PRESENCE OR ABSENCE OF CORONARY HEART DISEASE, WAS
MEASURED FOR 100 SUBJECTS PARTICIPATING IN A STUDY REPORTED BY
HOSMER AND LEMESHOW(1989). AFTER DETERMINING HOW TO PLOT THE DATA
WE WILL FIT A LOGISTIC REGRESSION OF CHD ON AGE;

OPTION NODATE;

DATA HEARTY;
INPUT AGE CHD @@;
LABEL AGE = 'AGE OF SUBJECT'
CHD = 'CORONARY HEART DISEASE STATUS';
IF AGE<30 THEN AGEGRUP=25;
ELSE IF AGE<35 THEN AGEGRUP=32;
ELSE IF AGE<40 THEN AGEGRUP=37;
ELSE IF AGE<45 THEN AGEGRUP=42;
ELSE IF AGE<50 THEN AGEGRUP=47;
ELSE IF AGE<55 THEN AGEGRUP=52;
ELSE IF AGE<60 THEN AGEGRUP=57;
ELSE AGEGRUP=65;

CARDS;
20 0 23 0 24 0 25 1 26 0 26 0 28 0 28 0 29 0
...
;

* THE VARIABLE AGEGRUP CONTAINS THE MIDPOINTS FOR THE AGE GROUPS.
IT WILL BE USED TO GIVE A PLOT THAT IS MUCH MORE INFORMATIVE THAN
THE RAW DATA PLOT;

PROC PLOT;
PLOT CHD*AGE;
```

```
TITLE 'THE RAW DATA PLOT: NOT VERY INFORMATIVE';
RUN;

PROC MEANS;
CLASS AGEGRUP;
VAR CHD;
OUTPUT OUT=NEW MEAN=CHDPROP;
TITLE 'USING THE MEANS PROCEDURE TO CALCULATE GROUP PROPORTIONS';
RUN;

PROC PRINT DATA=NEW;
TITLE 'OUTPUT DATASET CREATED BY THE MEANS PROCEDURE';
RUN;

DATA NEW;
SET NEW;
IF _N_=1 THEN DELETE;
DROP _TYPE_ _FREQ_;

PROC PLOT DATA=NEW;
PLOT CHDPROP*AGEGRUP='*';
TITLE 'PLOT OF GROUP PROPORTIONS AGAINST GROUP MIDPOINTS';
TITLE2 'NOTICE THE S-SHAPED PATTERN';
RUN;

PROC LOGISTIC DATA=HEARTY DESCENDING;
MODEL CHD=AGE;
TITLE 'LOGISTIC REGRESSION FOR CHD STATUS: AGE IS THE INDEPENDENT VAR';
RUN;

* NOTE: USE THE DESCENDING OPTION TO MODEL THE 1'S AND NOT THE 0'S;
```

11.19.2 Testing for Significance of the Coefficients

As in ordinary regression, when we fit the model, we would like to test independent variables for significance. In ordinary regression, this can be done with t of F tests which come from calculating the change in SS(E) for models with or without variables in question.

In logistic regression the idea is similar, but we do not work with sums of squares. Instead, we work with the likelihood function. We use the change in the log likelihood for the models with and without the variables. For a model with one independent variable, this is $L(\beta_0) - L(\beta_0, \beta_1) = \ln l(\beta_0) - \ln l(\beta_0, \beta_1)$. For theoretical reasons we multiply this by -2 to get: $G = -2\ln l(\beta_0) - (-2)\ln l(\beta_0, \beta_1)$. Under the hypothesis $\beta_1 = 0$, the distribution of G is approximately $\chi^2(1)$.

There are two other commonly used tests of significance for the independent variables:

1. The Wald test — The Wald test is analogous to the t-test in ordinary linear regression. It compares the MLE $\widehat{\beta}_1$ of the slope to an estimate of its standard error, but then squares the ratio to obtain a χ^2 with 1 degree of freedom. The Wald Chi-square is $\left(\frac{\widehat{\beta}_1}{s.e.(\widehat{\beta}_1)}\right)^2 = \frac{\widehat{\beta}_1^2}{s^2\widehat{\beta}_1}$. The $s.e.(\widehat{\beta}_1)$ calculation is based on an asymptotic expression. For small samples the likelihood ratio test above is preferable.

2. The Score test — The score test comes from the second likelihood equation: $\sum_{i=1}^n x_i[y_i - \Pi(x_i)] = 0$. If $H_0 : \beta_i = 0$ is true, then $\widetilde{\Pi}(x_i) = \bar{y}$ and so the left hand side of this equation becomes $\sum_{i=1}^n x_i(y_i - \bar{y})$

whose standard error is $\sqrt{\bar{y}(1-\bar{y})\sum_{i=1}^{n}(x_i-\bar{x})^2}$ The score test compares the value to its standard error. Squaring gives an approximate Chi-square. The score Chi-square is $\frac{\left[\sum_{i=1}^{n} x_i(y_i-\bar{y})^2\right]^2}{\bar{y}(1-\bar{y})\sum_{i=1}^{n}(x_i-\bar{x})^2}$

11.19.3 The Multiple Logistic Regression Model

Just as in ordinary regression, we can have multiple independent variables in a logistic regression model. If the independent variables are $x_1, x_2, ..., x_p$, then the multiple logistic regression model is $\ln\left(\frac{\Pi(x_i)}{1-\Pi(x_i)}\right) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_p x_{ip}$ or $\Pi(x_i) = \frac{e^{\beta_0+\beta_1 x_{i1}+\cdots+\beta_p x_{ip}}}{1+e^{\beta_0+\beta_1 x_{i1}+\cdots+\beta_p x_{ip}}}$. The x's can be continuous or categorical. Hence, we can have ANOVA-like models, regression-like models, and combinations of the two. For x's that are categorical, we have to create dummy variables just as we did for regression formulations of 1-factor and 2-factor experiments.

We wish to use the mle technique to estimate the β's. There will be $p+1$ likelihood equations obtained by differentiating the log likelihood with respect to each of the β's. After simplification, the equations become $\sum_{i=1}^{n} y_i - \Pi(x_i) = 0$, $\sum_{i=1}^{n} x_{ij}[y_i - \Pi(x_i)] = 0, i = 1, 2, ..., p$. These are solved computationally to get estimates $\widehat{\beta}_1, \widehat{\beta}_2, ..., \widehat{\beta}_p$ and hence $\widehat{\Pi}(x_i)$.

Tests for significance:

1. The overall test for regression $H_0 : \beta_1 = \beta_2 = \cdots = \beta_p = 0$ based on $G = -2\ln[l(\beta_0)] - [-2\ln l(\beta_0, \beta_1, ..., \beta_p)]$ is called the *likelihood ratio test statistic.* Reject H_0 if $G > \chi^2_\alpha(p)$.

2. A score test can be done. Stating the form of this test requires much complicated notation. So, we skip.

3. Wald tests for individual variables are as before. Calculate $\frac{(\widehat{\beta}_j)^2}{s^2(\widehat{\beta}_j)}$ and compare to $\chi^2_\alpha(1)$.

4. A general likelihood ratio test for throwing out a subset of variables, say $\beta_{k+1}, \beta_{k+1}, ..., \beta_p$ is $G = -2\ln l(\beta_0, \beta_1, ..., \beta_k) - [-2\ln l(\beta_0, \beta_1, ..., \beta_p)]$. $H_0 : \beta_{k+1} = \beta_{k+2} = \cdots = \beta_p = 0$. Reject H_0 if $G > \chi^2_\alpha(p-k)$.

SAS Code

```
FIRST EXAMPLE OF A MULTIPLE LOGISTIC REGRESSION. THE DATA IS FROM
A STUDY ON LOW INFANT BIRTH WEIGHTS. DETAILS ARE ON THE ACCOMPANYING
HANDOUT. HERE WE ILLUSTRATE MULTIPLE LOGISTIC REGRESSION BY FITTING
TWO DIFFERENT MODELS USING A FEW OF THE INDEPENDENT VARIABLES THAT
ARE AVAILABLE;

OPTION NODATE;

DATA LOWBIRTH;
INFILE 'BWT RAW A';
INPUT ID LOW AGE LWT RACT SMOKE PTL HT UI FTV BWT;
IF RACE=2 THEN RACE_1=1; ELSE RACE_1=0;
IF RACE=3 THEN RACE_2=1; ELSE RACE_2=0;

PROC LOGISTIC DESCENDING;
MODEL LOW=AGE LWT RACE_1 RACE_2 FTV;
TITLE 'THE FULL MODEL';
RUN;

PROC LOGISTIC DESCENDING;
MODEL LOW=LWT RACE_1 RACE_2/COVB;
```

```
TITLE 'THE REDUCED MODEL';
RUN;

* TO ASSESS THE JOINT CONTRIBUTION OF AGE AND FTV, CALCULATE(BY HAND)
THE DIFFERENCE IN THE -2 LOG L STATISTICS FOR THE TWO MODELS.
```

11.19.4 Lack-of-Fit

We investigate 3 basic methods for evaluating the fit of a logistic regression model. There is no R^2.

1. Evaluation relative to an expanded model. Suppose our current model has independent variables $x_1, x_2, ..., x_k$. Available but not in the model are $x_{k+1}, ..., x_p$. We may judge our model adequate if we are unable to improve it with the addition of other variables.

   In SAS, this can be done in 2 ways: 1) use PROC LOGISTIC to fit each model. The current model and then the model with $x_1, x_2, ..., x_p$. Then, calculate by hand $G = -2\ln l(\beta_0, \beta_1, ..., \beta_k) - [-2\ln l(\beta_0, \beta_1, ..., \beta_p)]$ and compare to $\chi^2(p-k)$. We studied this in the previous section. 2) Use of SELECTION=FORWARD in a model that INCLUDES $x_1, x_2, ..., x_k$ automatically. SAS generates a score test for comparing the model $x_1, x_2, ..., x_k$ only to the model with all available variables. There are no calculations by hand here.

2. Hosmer-Lemeshow Lack-of-Fit — Having fit the model, proceed as follow:

   (a) Form groups of observations based on decile of fitted probabilities, ie the observations with lowest 10% predicted probability in group 1, second lowest 10% group, etc to get 10 groups.

   (b) For each group, count how many of the observations have $y = 1$ and how many observations have $y = 0$.

   (c) For each group, calculate the expected number of observations with $y = 1$ and the expected number of observations with $y = 0$. For $y = 1$, just add the predicted probabilities.

   (d) Use a chi^2 test with $t - 2$ degrees of freedom to compare observed to expected. Here t is the number of groups.

   SAS implements this with the LACKFIT option. Depending on the number of observations, it may produce $t < 10$ groups.

3. Statistics for Comparing Models — The two statistics introduced here provide a way to compare different models for the same data while accounting for the number of independent variables p and the number of observations N.

   (a) AIC(Akaike's Information Criterion) is $-2\log L + 2(p+2)$.

   (b) SC(Schwartz's Criterion) is $-2\log L + (P+2)\log N$.

   For either one, smaller values are more desirable.

SAS Code

```
THE CHD DATA. MODELS ARE RUN, ALONG WITH THE LACKFIT OPTION;

OPTION NODATE;

DATA HEARTY;
INPUT AGE CHD @@;
LABEL AGE = 'AGE OF SUBJECT'
CHD = 'CORONARY HEART DISEASE STATUS';
IF AGE<30 THEN AGEGRUP=25;
```

```
ELSE IF AGE<35 THEN AGEGRUP=32;
ELSE IF AGE<40 THEN AGEGRUP=37;
ELSE IF AGE<45 THEN AGEGRUP=42;
ELSE IF AGE<50 THEN AGEGRUP=47;
ELSE IF AGE<55 THEN AGEGRUP=52;
ELSE IF AGE<60 THEN AGEGRUP=57;
ELSE AGEGRUP=65;

IF AGEGRUP=25 THEN Z1=1; ELSE Z1=0;
IF AGEGRUP=32 THEN Z2=1; ELSE Z2=0;
IF AGEGRUP=37 THEN Z3=1; ELSE Z3=0;
IF AGEGRUP=42 THEN Z4=1; ELSE Z4=0;
IF AGEGRUP=47 THEN Z5=1; ELSE Z5=0;
IF AGEGRUP=52 THEN Z6=1; ELSE Z6=0;
IF AGEGRUP=57 THEN Z7=1; ELSE Z7=0;

AGE2=AGE**2; AGE3=AGE**3; AGE4=AGE**4;
AGE5=AGE**5; AGE6=AGE**6; AGE7=AGE**7;
AGEGRUP2=AGEGRUP**2; AGEGRUP3=AGEGRUP**3; AGEGRUP4=AGEGRUP**4;
AGEGRUP5=AGEGRUP**5; AGEGRUP6=AGEGRUP**6; AGEGRUP7=AGEGRUP**7;

CARDS;
20 0 23 0 24 0 25 1 26 0 26 0 28 0 28 0 29 0
...
;

PROC LOGISTIC DATA=HEARTH DESCENDING;
MODEL CHD=AGE/LACKFIT;
TITLE 'LOGISTIC REGRESSION WITH AGE AS INDEPENDENT VARIABLE';
RUN;

PROC LOGISTIC DATA=HEARTY DESCENDING;
MODEL CHD=AGE AGE2 AGE3 AGE4/SELECTION=FORWARD INCLUDE=1 DETAILS;
TITLE 'USING FORWARD SELECTION TO EVALUATE RESIDUAL SCORE STATISTICS';
TITLE2 'EVALUATES LINEAR MODEL IN CONTEXT OF A 4TH DEGREE POLYNOMIAL';
RUN;

PROC LOGISTIC DATA=HEARTY DESCENDING;
MODEL CHD=Z1 Z2 Z3 Z4 Z5 Z6 Z7/LACKFIT;
TITLE 'SATURATED MODEL USING INDICATORS FOR GROUPED AGES';
TITLE2 'THIS IS LIKE A 1-FACTOR ANOVA IN CHPT 14 OF BOWERMAN-OCONNELL';
TITLE3 'BUT NOW THE DEPENDENT VARIABLE IS 0-1';
RUN;

PROC LOGISTIC DATA=HEARTY DESCENDING;
MODEL CHD=AGEGRUP AGEGRUP2 AGEGRUP3 AGEGRUP4 AGEGRUP5 AGEGRUP6 AGEGRUP7/LACKFIT;
TITLE 'SATURATED POLYNOMIAL MODEL FOR GROUPED AGES';
RUN;

* THESE LAST TWO PROC LOGISTICS DEMONSTRATE THAT, LIKE IN ORDINARY
REGRESSION, IF GROUPS ARE DEFINED BY A NUMERIC VARIABLE, WITH I VALUES,
THEN FITTING AN I-1 DEGREE POLYNOMIAL IS EQUIVALENT TO USING I-1
INDICATORS. IN THE LOGISTIC REGRESSION SETTING, A MODEL WHICH CONTAINS
A PARAMETER FOR EVERY LEVEL OF THE GROUPING VARIABLE IS SAID TO BE
```

```
"SATURATED.";
```

11.19.5 Interpreting the Regression Coefficients

Interpreting the coefficient involves 2 issues:

1. Determining the functional relationship between the dependent variable and the independent variable.
2. Appropriately defining the unit of change for the independent variable.

For instance, with the simple logistic regression with only one independent variable $g(x) = \ln\left(\frac{\Pi(x)}{1-\Pi(x)}\right) = \beta_0 + \beta_1 x$ where $g(x)$ is the logit transform. Then $\beta_1 = g(x+1) - g(x)$ is the change in the logit for unit change in x.

1. Categorical Dictonomous Independent Variables — A *dictonomous variable* only has two categories.

   Example: $age < 55$, $age \geq 55$.

   With two categories, we need 1 dummy variable with values 0 and 1. So,

   $$g(1) = \ln\left(\frac{\Pi(1)}{1-\Pi(1)}\right), \;\; g(0) = \ln\left(\frac{\Pi(0)}{1-\Pi(0)}\right), \;\; \beta_1 = g(1) - g(0) = \ln\left(\frac{\frac{\Pi(1)}{1-\Pi(1)}}{\frac{\Pi(0)}{1-\Pi(0)}}\right).$$

   which is called the *log odds ratio.* The *odds ratio* is given by $e^{\beta_1} = \frac{\frac{\Pi(1)}{1-\Pi(1)}}{\frac{\Pi(0)}{1-\Pi(0)}}$. The confidence interval for the odds ratio is $e^{\widehat{\beta} \pm z_{\alpha/2} s.e.(\widehat{\beta})}$. The group in the denominator is called the *reference group.*

2. Polytomized Independent Variable — When an independent variable is categorical with more than 2 groups, it is said to be *polytomious.* If there are k categories, we need $k-1$ indicators(dummy variables) for the logistic model. Our model is

   $$g(z) = \ln\left(\frac{\Pi(z)}{1-\Pi(z)}\right) = \beta_0 + \beta_1 z_1 + \beta_2 z_2 + \cdots + \beta_{k-1} z_{k-1}$$

   where $z_1, z_2, ..., z_{k-1}$ are indicators defined in the usual way. The group that does not have an indicator is called the *reference group.* We seek meaning to $\beta_1, \beta_2, ..., \beta_{k-1}$. Consider $\mathbf{Z} = (z_1, z_2, ..., z_{k-1})$ Then, $z_1 = (1, 0, ..., 0)$. $z_0 = (0, 0, ..., 0)$. $g(z_1) - g(z_0) = (\beta_0 + \beta_1) - \beta_0 = \beta_1$. $beta_1$ is the log odds ratio for group 1 relative to group k. β_2 is the log odds ratio for group 2 relative to group k. Thus, e^{β_1} is the odds ratio for group 1, etc. The odds ratio for comparing group j to group j' is $e^{\beta_j - \beta'_j}$.

3. Continuous Independent Random Variable — The equation for the logit is

   $$g(x) = \ln\left(\frac{\Pi(x)}{1-\Pi(x)}\right) = \beta_0 + \beta_1 x.$$

   From that

   $$\beta_1 - g(x+1) - g(x) = \ln\left(\frac{\frac{\Pi(x+1)}{1-\Pi(x+1)}}{\frac{\Pi(x)}{1-\Pi(x)}}\right)$$

   which is the log odds ratio for comparing individuals separated by 1 unit of x. The estimate is $e^{\widehat{\beta}_1}$. The confidence interval is $e^{\widehat{\beta}_1 \pm z_{\alpha/2} s.e.(\widehat{\beta}_1)}$. CAUTION: Does a 1 unit change in x have meaning? Sometimes yes and sometimes no.

4. Multivariate Case(No Interaction) — Take the low birth rate data. Consider the model with LWD(x_1) and age(x_2). The model is

$$\ln\left(\frac{\Pi(x_1,x_2)}{1-\Pi(x_1,x_2)}\right) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 = g(x).$$

Then, $g(1,x_2) - g(0,x_2) = (\beta_0 + \beta_1 + \beta_2 x_2) - (\beta_0 + \beta_2 x_2) = \beta_1$.

$$\beta_1 = \ln\left(\frac{\frac{\Pi(1,x_2)}{1-\Pi(1,x_2)}}{\frac{\Pi(0,x_2)}{1-\Pi(0,x_2)}}\right)$$

is the odds ratio for comparing the low-last weight group to the high last weight group adjusting(accounting) for age. x_2 must be kept fixed. Vary x_1 by 1 unit.

More generally, for a model with independent variables $x_1, ..., x_p$

$$Y(x) = \ln\left(\frac{\Pi(x)}{1-\Pi(x)}\right) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p.$$

β_i is the log odds ratio for a unit change in x_i holding the other $x's$ fixed.

5. Multivariate Case with Interaction — What distinguishes the interaction case from the no-interaction case is no interaction can change the variable of interest while keeping other variables fixed. In the interaction model, changing the variable of interest changes other variables, also.

SAS Code

```
MODEL-FITTING WITH THE LOW BIRTHWEIGHT DATA;


OPTION NODATE;

DATA LOWBIRTH;
INFILE 'BWT RAW A';
INPUT ID LOW AGE LWT RACT SMOKE PTL HT UI FTV BWT;
IF RACE=2 THEN RACE_1=1; ELSE RACE_1=0;
IF RACE=3 THEN RACE_2=1; ELSE RACE_2=0;

IF LWT<110 THEN LWD=1; ELSE LWD=0; *DICHOTOMIZING;
IF PTL>0.5 THEN PTD=1; ELSE PTD=0; *DICHOTOMIZING;

* THE FOLLOWING ARE POSSIBLE 2-WAY INTERACTION TERMS;

R1LWD=RACE_1*LWD; R1SMOKE=RACE_1*SMOKE; R1PTD=RACE_1*PTD;
R1HT=RACE_1*HT;
R2LWD=RACE_2*LWD; R2SMOKE=RACE_2*SMOKE; R2PTD=RACE_2*PTD;
R2HT=RACE_2*HT;

LWDSMOKE=LWD*SMOKE; LWDPTD=LWD*PTD; LWDHT=LWD*HT;
SMOKEPTD=SMOKE*PTD; SMOKEHT=SMOKE*HT; PTDHT=PTD*HT;

* WE WILL EXAMINE TWO-WAY TABLES TO ASSESS THE MARGINAL BENEFIT OF
EACH VARIABLE. THIS IS ANALOGOUS TO INITIAL PLOTS OF Y VERSUS X
IN ORDINARY REGRESSION;
```

```
PROC FREQ;
TABLES LWD*LOW RACE*LOW SMOKE*LOW PTD*LOW HT*LOW
UI*LOW FTV*LOW/NOCOL NOPERCENT CHISQ;
TITLE 'TWO-WAY TABLES: DEPENDENT AGAINST EACH PREDICTOR';
RUN;

PROC LOGISTIC DESCENDING;
MODEL LOW=RACE_1 RACE_2 AGE LWD SMOKE PTD HT UI FTV/INCLUDE=2
SELECTION=STEPWISE SLENTRY=.15 LSSTAY=.20;
TITLE 'STEPWISE SELECTION WITH RACE INCLUDED';
RUN;

PROC LOGISTIC DESCENDING;
MODEL LOW=RACE_1 RACE_2 AGE LWD SMOKE PTD HT UI FTV/
SELECTION=BACKWARD SLSTAY=.20;

TITLE 'BACKWARD SELECTION';
RUN;

PROC LOGISTIC DESCENDING;
MODEL LOW=RACE_1 RACE_2 LWD SMOKE PTD HT
R1LWD R1SMOKE R1PTD R1HT
R2LWD R2SMOKE R2PTD R2HT
LWDSMOKE LWDPTD LWDHT
SMOKEPTD SMOKEHT PTDHT/INCLUDE=6
SELECTION=FORWARD;
TITLE 'TRYING INTERACTION TERMS/CALCULATION OF RESIDUAL SCORE STATISTIC';
RUN;


PROC LOGISTIC DESCENDING;
MODEL LOW=RACE_1 RACE_2 LWD SMOKE PTD HT
R1LWD R1SMOKE R1PTD R1HT
R2LWD R2SMOKE R2PTD R2HT
LWDSMOKE LWDPTD LWDHT
SMOKEPTD SMOKEHT PTDHT/INCLUDE=6
SELECTION=STEPWISE SLSTAY=.20 SLENTRY=.15;
TITLE 'STEPWISE INVESTIGATION OF TWO-WAY INTERACTION TERMS';
RUN;

PROC LOGISTIC DESCENDING;
MODEL LOW=RACE_1 RACE_2 LWD SMOKE PTD HT
R1LWD R2LWD R1SMOKE R2SMOKE LWDHT/INCLUDE=6
SELECTION=FORWARD DETAILS;
TITLE 'RESIDUAL SCORE STATISTIC FOR A SUBSET OF INTERACTIONS';
RUN;

PROC LOGISTIC DESCENDING;
MODEL LOW=RACE_1 RACE_2 LWD SMOKE PTD HT
R1LWD R2LWD;
TITLE 'RACE-LWD INTERACTION ONLY';
RUN;
```

```
PROC LOGISTIC DESCENDING;
MODEL LOW=RACE_1 RACE_2 LWD SMOKE PTD HT
R1SMOKE R2SMOKE;
TITLE 'RACE-SMOKE INTERACTION ONLY';
RUN;

PROC LOGISTIC DESCENDING;
MODEL LOW=RACE_1 RACE_2 LWD SMOKE PTD HT
LWDHT;
TITLE 'LWD-HT INTERACTION ONLY';
RUN;

PROC LOGISTIC DESCENDING;
MODEL LOW=RACE_1 RACE_2 LWD SMOKE PTD HT /LACKFIT;
TITLE 'THE MAIN EFFECTS MODEL';
RUN;
```

11.20 References

Homser and Lemeshow (1989), *Applied Logistic Regression,* Wiley.

Chapter 12

Clinical Trials

Dr. Lee, Old Dominion University

STAT 540, Spring 1997

Text used: Friedman, L. M., C. D. Furberg, and D. L. DeMets, *Fundamentals of Clinical Trials, 3-rd edition,* 1996

12.1 Outline

1. Definition and types of trials.
2. Clinical trial phases.
3. The study protocol.
4. Essentials of good clinical trial design.
5. Brief history of clinical trials.
6. Defining the study population.
7. Four major study designs: their strengths and weaknesses.
8. Methods of randomization: simple, blocked, stratified.
9. Baseline assessment.
10. Blinding or masking of treatment assignments.
11. Monitoring compliance.
12. Exclusions, withdrawals, losses: which subjects should be included in the analysis of trial results?

A clinical trial is a prospective study of the effects of one or more test treatments and a control treatment on human subjects. It is generally accepted that a randomized controlled trial is the most reliable method of conducting clinical research. The subjects are enrolled, treated, and followed forward in time; however, they need not all enter the trial simultaneously, and in fact, patients often enter the trial at different times. The outcome measure may be death, a non-fatal clinical event or a laboratory test. The time period of the trial may be short or long, depending on the outcome measure. In the phases, the historical controls include 1) animal studies, 2) healthy volunteers, and 3) borderline individual case studies. Under this definition, studies that use a historical control group do not qualify as a clinical trial. Experiments on healthy human volunteers are borderline in that they provide only indirect evidence of the effect of a treatment. An individual case study, wherein one individual's pattern of treatment and response is reported as an interesting occurrence, also does not constitute a clinical trial. This is because other patients with the same condition will almost certainly show varied responses to the same treatment. That is, the experience of one patient does not adequately enable an inference to be made about the effect of treating future patients in the same way. One of the main problems in conducting a trial is getting a large enough group of patients on different treatments to make reliable treatment comparisons. There are various ways of classifying clinical trials. One way is by the type of treatment. The great majority of clinical trials are concerned with evaluation of drug therapy. However, clinical trials may also be concerned with surgical procedures, radiation treatments, and different forms of medical advice (e.g. diet and exercise). The treatments used in clinical trials are often called interventions and are classified as follows:

1. Prophylactic — a treatment aimed at preventing the development of a disease or condition (e.g. a new vaccine).
2. Therapeutic — a treatment aimed at curing or healing a disease or condition (e.g. drugs, devices, procedures).
3. Diagnostic — identifying the sign or symptoms by which a disease is known (e.g. an AIDS test).

12.1.1 Clinical Trial Phases

The process of running clinical trials to qualify a new drug for sale to the public has been classified by the FDA into the following three phases:

1. Phase I Trial (Early) — Determine whether there is a dosage regimen not overly toxic and suitable for further study of therapeutic effect. The sample size is usually 4-10 subjects and lasts no more than 20-80 days. In this design, select healthy volunteers who are given a new drug; observations are made; then a washout period; the subject is then given the next drug in the same manner; order of receiving the drugs is randomized.
2. Phase II Trial (Efficacy) — Estimate the effectiveness of the regimen after passing a preliminary trial. The sample size is usually 20-80 subjects; usually no more than 150-200 subjects; In this design, the features are controlled; double-blinded; monitored; and randomized.
3. Phase III Trial (Effectiveness) — Compare the effectiveness of the new treatment with a standard or control treatment. The sample size is usually several thousand subjects.

Efficacy refers to what the treatment will accomplish in an ideal setting where all participants are eligible to receive the treatment and comply perfectly with the assigned treatment and treatment schedule. Effectiveness refers to what the treatment will accomplish in actual practice. For example, if 60% of the patients respond favorably to a new treatment under ideal conditions, then the treatment efficacy is a 60% success rate. Our text (Chapter 14) emphasizes the importance of analyzing the trial results in ways that reflect the treatment effectiveness.

12.1.2 The Study Protocol

A written protocol must document the purpose, design, and conduct of a clinical trial. It must be specific with respect with respect to which patients are to be included and excluded from the trial, the treatments to be tested, the outcome measures, etc. The following list is a brief outline of a protocol document.

1. Background of the study.
2. Objectives
   (a) Primary question and response variable.
   (b) Secondary questions and response variables.

   (c) Sub-group hypotheses.

3. Design of the study.
   (a) Study population.
      i. Inclusion and exclusion criteria.
      ii. Sample size estimates.
   (b) Enrollment of subjects.
      i. Informed consent.
      ii. Assessment of eligibility.
      iii. Baseline examination.
      iv. Treatment allocation.
   (c) Intervention (i.e. treatment).
      i. Description and schedule.
      ii. Measures of compliance — want this to be high.
   (d) Follow-up visit description and schedule.
   (e) Ascertainment of response variables.
      i. Training.
      ii. Data collection.
      iii. Data monitoring and quality control.
      iv. Data analysis.
   (f) Organization.
      i. Participating investigators.
      ii. Study administration.
         A. Committees and sub-committees.
         B. Policy and data monitoring committee.

12.1.3 Essentials of Good Clinical Trial Design

This section comes from Wooding, Planning Pharmaceutical Clinical Trials, 1994. There are many features of a good trial design that are important, but there are three that should always be present, except in rare cases.

1. The use of concurrent controls (a placebo, a standard treatment, or both).
2. Double-blinding.
3. Randomization.

A trial lacking any of these features is likely to be rejected by the FDA and will be unconvincing to other informed critics such as journal readers. The use of before and after tests, that omit concurrent controls and use only baseline data, is not an acceptable substitute for concurrent controls. One reason for this is that baseline responses may change from one time period to another, even in the absence of a treatment effect.

12.1.4 The History of Clinical Trials

The modern era of properly designed clinical trials begins about 1950. Before this time, most trials did not involve a control group or randomization. By 1950, or shortly thereafter, most of the ground rules for conducting clinical trials on a scientific basis had been established. The concept of multiple investigators, different study sites, and a common study protocol emerged in the 1930's. The first trial with a properly randomized control group (1948) studied streptomycin as a treatment of pulmonary tuberculosis. The U.S.

polio vaccine trials began in 1953 and involved thousands of volunteers and a placebo group. One of the first multi-center, randomized trials in the U.S. was the University Group Diabetes Program (1961 - 1974). It involved seven clinics, four treatment groups, and a sample size over 1,000 patients. In 1969, the FDA began requiring evidence from a randomized controlled trial to gain approval for marketing a new drug. It was only in the mid 1970's that properly done clinical trials began to be widespread in the pharmaceutical industry. Any clinical trial requires a clear definition of which patients are eligible for inclusion and also a list of exclusion criteria to supplement the main definition of the disease. The study population is a subset of the general population defined by the inclusion-exclusion criteria. Usually, subjects are not randomly chosen from the study population. Judgments about whether the study results can be generalized from the subjects actually in the trial to the study population can be made from defined medical conditions and by observing explanatory variables such as age, sex, elevated blood pressure, etc. The impact of the eligibility criteria on the recruitment of patients should be considered when deciding on these criteria. Excessive restrictions implies extreme difficulty in recruiting an adequate number of participants.

12.1.5 General Criteria for Inclusion and Exclusion

1. Include those patients most likely to benefit from the treatments being studied (those that have the disease being studied and those that are likely to respond to treatment). Knowing the mechanism of action of a treatment enables an investigator to identify those subjects most likely to respond to treatment. For example, type of bacteria and site of an infection enables determining whether a new antibiotic may be effective in treating a urinary infection. If the mechanism of action of a treatment is unclear or if there is uncertainty about the stage of the disease at which a treatment may be most beneficial, then the subjects that are most likely to respond to the treatment cannot easily be selected. An unknown mechanism of action implies a) a more heterogeneous study population, b) a reduced chance of detecting a treatment difference.

2. Include those subjects for which there is a high likelihood of detecting a treatment difference. If the primary response variable is continuous (e.g. blood pressure, serum cholesterol level, etc) change is easier to detect if the initial level is extreme. For example, one would expect a more pronounced drop in blood pressure in a subject with an initial systolic blood pressure of 135mm of Hg than in a subject with an initial BP of 125mm of Hg. Subjects with frequent cardiac arrhythmic episodes are more likely to respond to an anti-arrhythmic agent than subjects with only one brief episode.

3. Exclude any subject for which a treatment is known to be harmful. Pregnant women are often excluded from drug trials unless the primary question concerns pregnancy. People with a history of gastric bleeding are usually excluded from trials of almost any anti-inflammatory drug. These exclusions apply only before the enrollment of a subject in a trial; participants my develop conditions during a trial which would have excluded them had the conditions been present earlier. In these circumstances, a participant may be removed from a treatment but kept in the trial for the purpose of analysis.

4. Exclude subjects at high risk of developing conditions that preclude observing the event of interest. People with cancer or severe kidney disorders are usually excluded from trials in which the primary question concerns heart disease, as they may die or withdraw from the study before the primary response variable can be observed. When there is a competing risk, the ability to assess a treatment effect is decreased and biased results may be obtained for the primary study question if the treatment in some way has a harmful or beneficial effect on the co-existing condition.

5. Include only those subjects who are likely to comply with the assigned treatment and treatment schedule. Non-compliance reduces the opportunity to observe the effect of a treatment. Unfortunately, there is no way to guarantee that a given subject will comply.

12.1.6 Example of Selection Criteria

This example of selection criteria of patients comes from the study of chemotherapy trial for advanced colorectal cancer (Pocock, 1983).

1. Patients must have histologically confirmed metastic or locally recurrent carcinoma of the colon of the rectum.

2. The tumor must be beyond hope of surgical eradication.

3. The tumor masses must be measurable by physical examination or chest x-ray.

4. No previous chemotherapy treatment for the disease.

5. Expected survival of at least 90 days and absence of severe malnutrition, nausea, and vomiting.

6. If the white blood cell count is too low, then the patient can not tolerate chemotherapy. The white blood cell count should be greater than 4,000 per mm^3. The platelet count should be greater than 100,000 per mm^3. The haemoglobin should be greater than 10 grams per 100 ml. The creatinine should be less-than 1.5 mg per 100 ml.

12.1.7 Baseline Assessment

Baseline refers to the status of a patient before he is randomized to a treatment group. Baseline data may be collected by interview, questionnaire, physical exam, and laboratory tests. These include personal characteristics (e.g. age, sex) and clinical history (e.g. duration of illness and previous therapy); includes measurable parameters that may change during the trial (e.g. blood pressure, tumor size, Hamilton rating of depression). The following lists the uses of baseline measurements.

1. To determine patient eligibility.

2. To characterize the population to which the results of the trial may be generalized.

3. To identify subgroups of patients for which a treatment may have a beneficial or harmful effect.

4. To stratify the patients at the time of randomization or during the analysis of trial results.

Problem 1: A patient's baseline status may change before the initiation of treatment. By definition, a baseline measurement is any measurement taken at or before randomization. Any change in a baseline measurement that occurs after randomization is usually regarded as an outcome of the trial and is, therefore, not a baseline measurement. A patient's baseline status may change between the time of randomization and the time that the treatment begins. For example, a patient's diastolic blood pressure may drop from 95 mm of Hg to 85 mm of Hg. Such a change may dilute the results of the trial and thus decrease the chance of detecting a treatment difference. Another example, a new antihypertensive agent would not produce as large of a decrease in dbp as it would have in the baseline value where higher. Possible solution: wait until the latest possible moment to randomize each patient.

Problem 2: Observer variation. Some clinicians and nurses record consistently higher or lower blood pressure values than others. Possible solutions: use training sessions; take repeated measurements on each subject using two or three different observers and record the average.

Problem 3: Objective assessment. Example: three cardiologist were asked to interpret the same ECGs for 1,252 patients suspected of heart disease. They disagreed in 132 cases on whether the patient had an infarct (Pocock, 1983). Possible solutions: use an objective classification of ECGs; use a panel of two or three observers to resolve the differences.

12.1.8 Four Major Study Designs

1. The randomized controlled design. Patients are randomly allocated to treatment and control groups.

2. Non-randomized concurrent controls. One group is given a standard treatment at approximately the same time as another group receiving the new treatment. For example, the survival time is compared for patients in each of two different hospitals where one hospital is using a new surgical technique and the other is using traditional care.

3. Historical controls. A new treatment is used on a current set of patients and the results are compared to those obtained at a different point in time for a "comparable" group of patients that received a standard treatment.

4. Cross-over design. Patients are randomized to 2 groups. Patients assigned to one group first receive treatment A and then later receive treatment B. Patients in the other group receive B followed by A. This design uses small sample sizes because of "within" variability.

The following table lists the strengths and weaknesses of the four study designs.

Study Design	Strengths	Weaknesses
Randomized Control Design	Removes potential bias when randomly allocating subjects to the two groups.	Investigators as well as patients may be reluctant to place a patient in the (perceived) inferior treatment group.
	Tends to produce comparable groups since biases average out over the two groups.	For rare diseases it may be difficult to find an adequate number of patients for a randomized control study.
Non-randomized concurrent controls	The design is easier to use since one selects the treatment group and tries to match characteristics with a control group.	The treatment and control group may not be directly comparable. The burden of proof falls on the investigator to show that appropriate matching has been done (very difficult to do).
Historical Controls	No patient is denied access to a new therapy.	It is difficult, if not impossible to obtain a control group comparable to the treatment group in all ways except for the new treatment regimen. Historical records may be difficult to obtain; population characteristics (e.g. diet) may change over time.
	Roughly half as many patients are needed as in a randomized controlled study.	
The Cross-Over Design	Requires fewer patients to achieve the same power as a similar parallel groups design.	The effect of the treatment may carry over into the second period. Thus, results of the trial are considered more difficult to interpret than for a parallel groups design.

12.1.9 Methods of Randomization

1. Fixed allocation randomization. Fixed allocation procedures assign the study subjects (usually equally) to the treatment groups with fixed probabilities. The allocation probability does not change during the course of the trial. Some researchers advocate allocation procedures that are not 50:50. For example, Peto, et. al. (1976) recommend that sometimes a 2:1 allocation ratio, treatment-to-control be used. The rationale is that more information may be desired about a new treatment than about a control group. However, the general view is that 50:50 is more in keeping with the attitude of indifference toward which of the two groups a patient will be assigned. PROBLEM: Suppose the recruitment goal of a trial is 200 patients which are to be randomly and equally allocated to treatments A and B . Only about 30 of the patients have been identified and the remaining 170 will be recruited at a rate of about 4 per week. As a member of a design committee, you have been asked to develop a randomization schedule that ensures the following: a) a balanced assignment in case the trial terminates earlier than scheduled, and b) clinic personnel nor patients will be able to predict the next assignment (otherwise, patients with a good prognosis might be deliberately placed on a particular treatment and thus bias the results).

2. Simple Randomization. When a patient becomes eligible to be randomized, he may be assigned to a treatment by the toss of a coin or by a selection from a random number table. The main disadvantage of simple randomization is that a large imbalance may occur, especially in small trials. For example, with $N = 20$ subjects to be randomized, the chance of a 12:8 split or worse is about 0.50. With $N = 100$ subjects to be randomized, the chance of a 60:40 split or worse is about 0.05. Although imbalances are unlikely in large trials, there could be a serious imbalance if the trial ends earlier than scheduled.

3. Blocked randomization. Blocked randomization is used to avoid an imbalance in the number of subjects assigned to each group. Blocked randomization guarantees that at no time during the entry of patients into a trial will the imbalance be large. If equal allocation is used and subjects are randomly assigned to groups A and B, then for each block of even size (e.g. 4, 6, 8) exactly one-half of the subjects will be assigned to A and the other half to B. Within blocks the order in which treatments A and B are assigned to individual patients is randomized. This process is repeated for consecutive blocks of subjects until all subjects have been randomized. The smaller the block size the more likely it becomes that an investigator may discover blocking pattern and delay enrolling the next patient until, in his own judgment the "right" patient comes along. **Notation:** Let k be the number of treatment groups, and b be the block size (i.e. number of patients included in each block). The block size is greater than 2. The block size must be at least as large as k.

   Example 1: Develop a randomization schedule for assigning the first 4 patients to one of two treatments (say A and B) using equal allocation and a block size of 4. SOLUTION: Number the patients according to the time order in which they become available (1, 2, 3, 4). Note that there are 6 possible permutations of AABB, $\frac{4!}{2!2!}$. Make a list of these 6 permutations and number them 1-6. Select a number from the random number table that falls in the range 1-6. The result identifies the particular order (i.e. permutation) in which the treatments are assigned to the 4 patients.

   Example 2: For the next block of 4 patients a second number is selected from the random number table to randomly allocate the next 4 patients to the 2 treatments. Assuming that the entries from the random number table are 2 and 5, give the treatment assignment of the first 8 patients. What is the maximum imbalance that could occur if the trial ends earlier than scheduled?

   Example 3: Repeat Example 1 using a block of size 6.

   Example 4: Repeat Example 3 using an allocation ratio 2:1, A:B. Use a block of size 6. What is the maximum imbalance that could occur?

4. Stratified Randomization. *Stratification* refers to grouping the subjects on the basis of baseline measurements. Grouping done at or before randomization is called *pre-stratification.* Grouping done after randomization (usually at the analysis stage) is called *post-stratification.* Blocking, as described earlier, is a form of stratification with patients being grouped by time of entry into a trial. Variables with error prone classifications or subjective interpretations should not be used to form strata. Pre-stratification is primarily used in small to moderate sized trials where it is more likely that an imbalance may occur. For example, a large number of good prognosis patients may, by chance, be assigned to treatment #1 and a much smaller number to treatment #2. The main purpose of pre-stratification is to ensure comparable treatment groups. Pre-stratification is usually unnecessary in large trials because an imbalance is unlikely to occur. It is generally recommended that pre-stratification be used in multi-center trials where patients are grouped naturally by center or clinic. Stratified randomization proceeds in much the same way as described earlier. Blocking within strata is done with patients identified by time of entry within strata.

Example 5: This is an example of a stratified randomization with a block size of 4.

Age	Sex	Systolic Blood Pressure
(1) 40-49	(1) Male	(1) Greater than 130
(2) 50-59	(2) Female	(2) Less than or equal to 130
(3) 60-69		

The number of strata is $3 \times 2 \times 2 = 12$. So, number the strata 1 through 12. Subjects within stratum #1 become available in the time order 1, 2, ...

12.1.10 Blinding or Masking of Treatment Assignment

Blinding refers to the condition where knowledge of the treatment assignment is withheld from some individual or group of individuals. The purpose of blinding is to improve the objectivity of the data collection, reporting, and analysis process. It is important to use blinding when the outcome measures are subject to interpretation errors. Laboratory tests should be performed by personnel who are blinded to the treatment assignment. The only exception is those cases where the treatment assignment is needed to determine the test to be performed. ECGs, x-rays, and other photographs should be read by individuals blinded to the treatment assignment. Blinding should not be used if the study participant assumes a measurable risk in order to achieve or maintain blinding. Blinding is feasible only when it is possible to administer all treatments in an identical fashion and the clinic personnel do not need to know the treatment to care for the patient receiving it. A *single blind trial* is one in which only the participant does not know his treatment assignment. A *double blind trial* is one where neither the participant nor the investigator responsible for following the participant know the identity of the treatment assignment. A *triple blind trial* is one where neither the participant, nor the investigator, nor the committee responsible for monitoring response variables know the identity of the treatment assignment. Blinding is often used in drug trials and is difficult to use in trials where the treatment is invasive (e.g. surgery).

12.1.11 Monitoring Compliance

The term *compliance* refers to the extent to which a participant adheres to the assigned treatment, treatment schedule, and follow-up schedule of clinic visits e.g. takes medication at the prescribed dosage and frequency. Reasons for noncompliance include side effects, unwillingness to change behavior, not understanding instructions, condition deteriorates, etc. Noncompliance dilutes the treatment effect and may have a major effect on the power of the trial. A low level of compliance may be caused by inept planning and execution of the trial. Steps that can be taken before enrollment to minimize compliance problems include:

1. Exclude people addicted to drugs or alcohol, those who live too far from the clinic, and those likely to move before termination of the trial.
2. Exclude those that have concomitant diseases and are taking other medications.
3. Ensure that each participant is clearly instructed on the purpose of the trial and what is expected of him.
4. When feasible, before randomization use a run-in period to identify poor compliers and exclude them from the trial. A run-in period is also useful for detecting drug intolerance. The number of participants eliminated by the run-in period is usually small (5-10%). In 1988, a total of 26 trials used a run-in phase.

Steps that can be taken after randomization to maintain compliance include the following list.

1. Use special pill dispensers that help the participant keep track of when he has taken his medication.
2. Use counselors, physicians, and brochures to inform and encourage the participant to comply with his assigned treatment.
3. Have clinic staff remind the participant of upcoming visits.

Even if all of the above steps have been taken, we must still monitor and assess the level of compliance. The study protocol usually specifies that the level of compliance be monitored. Assessment of compliance level is needed to publish the study results.

Problem: As a member of a monitoring committee you have been asked to indicate the frequency and type of data to be collected to monitor patient compliance with the treatment and treatment schedule. A goal of the trial is a compliance rate of at least 90%. The committee wants to track the compliance rate in the two treatment groups and also monitor any trends in the compliance rates. In drug trials, pill or capsule count is the easiest and most commonly used measure of compliance. Laboratory results (e.g. blood and urine tests) are sometimes used but usually indicate only what has happened in the preceding one or two days.

Example : Consider the tablet compliance rate in the aspirin myocardial infarction trial.

	Ave. # of tablets Prescribed per Day		Ave. # of tablets Taken per Day		Ave. Percentage Compliance	
Visit	Group A	Group B	Group A	Group B	Group A	Group B
1	1.95	1.94	1.91	1.89	97.9	97.4
2	1.93	1.90	1.82	1.78	94.3	93.7
3	1.92	1.89	1.83	1.80	95.3	95.2

Example: Consider (a different trial) of aspirin compliance as indicated by salicylate level in urine tests. The following table of data was collected.

	Percentage of Participants Showing Positive Tests	
Visit	A (aspirin)	B (placebo)
1	88.5	3.0
2	86.1	4.4
3	86.8	4.2

12.1.12 Exclusions, Withdrawals, and Losses

Even if a trial is carefully planned, some participants may be lost to follow-up, not comply with the study protocol (i.e. deviate from the4 assigned treatment or treatment schedule), or perhaps not even have met the entrance requirements. Some investigators prefer to remove from the analysis those participants who do not meet the inclusion criteria or who do not follow the study protocol perfectly. Others believe that once a subject is randomized, he should always be followed and included in the analysis in the group to which he was randomly assigned. The latter point of view is widely accepted and is called an *analysis by intent to treat.*

Exclusions

Exclusions are people who are screened as potential trial participants, but who do not meet the entrance criteria and are therefore not randomized. Individual physicians may have, for certain of their patients, a definition preference for one or the other of the trial treatments. When this happens, the subject cannot ethically be admitted to the trial. He must be excluded from the trial and be given the treatment thought best for him, even if there is little objective basis for this preference. The trial protocol should contain specific instructions against randomizing patients who:

1. Are unlikely to tolerate one or more of the treatments.
2. Are extremely young or extremely old for the disease.
3. Seem unlikely to cooperate.
4. Live so far away that regular treatment may prove difficult.
5. Have a disease likely to take an abnormal course.

Exclusions, whether for whimsical or serious reasons, do not bias the treatment-control comparisons. They do influence the interpretation of th trial results by limiting the study population to which the results can be generalized.

Withdrawals

Withdrawals are randomized participants who are deliberately excluded from the analysis of trial results. The most common reasons for withdrawals are 1) the patient is found ineligible after he has been randomized (e.g. by miss diagnosis), 2) the patient does not comply with the assigned treatment or treatment schedule. The decision not to comply with the treatment or treatment schedule may be made by the participant, his primary care physician, or a trial investigator. Noncompliance may occur because of adverse effects of the treatment, loss of participant interest, changes in the condition of the participant, and a variety of other reasons. To minimize the number of randomized participants who are later found ineligible, Peto, et. al. (1976) suggest the following: 1) wait until the latest possible moment to randomize a patient, and 2) do not randomize a patient unless a diagnosis is unequivocal. Since withdrawals, for any reason, can bias the treatment-control comparisons, the ideal policy is to accept withdrawals under any circumstances. This uses the intent to treat philosophy. This policy may not be satisfactory if diagnosis of the disease is difficult. In such cases, Peto, et. al. (1976) suggest randomizing some or all of the patients whose diagnosis is doubtful and then withdraw any patient who is later proved to have the wrong disease.

Losses

Losses are randomized patients who are lost to follow-up. Losses may occur because the therapy was not successful or because it has been completely successful. There is no completely satisfactory way to account for such losses so do not let it happen. Patients who move away from the tral centers where they were admitted should still be followed when survival time is the main response variable. Losses can bias the treatment-control comparisons so every effort should be made to minimize losses.

12.1.13 Treatment Efficacy and Effectiveness

Some investigators argue that non compliers should be withdrawn from the analysis because otherwise the trial is not a fair test of a new treatment. That is, the treatment-control difference may be less that what it would have been if all patients had complied with the assigned treatment. To adjust for compliance, subgrouping is sometimes used to analyze treatment efficacy. However, many investigators believe that subgrouping on the basis of compliance level, withdrawing non compliers, or including them only up to the date at which they fail to comply with the assigned treatment is seriously wrong. Compliance level is an outcome of the trial and is therefore not considered to be an appropriate basis for subgrouping.

Example: Consider the coronary artery bypass surgery trial (1979). It was a randomized trial that compared bypass surgery to medical therapy in terms of the effect on mortality. After randomization, some of the patients were switched from medical treatment to surgery or from surgery to medical treatment. Critics of the trial argued that when the trial was started, the surgical techniques were still evolving. Thus, surgical mortality in the study did not reflect what occurred in actual practice at the end of this long-term trial. In addition, there were wide differences in surgical mortality between the cooperation clinics, which may have been related to the experience of the surgeons. The following table shows the two year mortality versus compliance levels.

	Treatment Group			
	Medical		Surgery	
	Received Medicine	Switched to Surgery	Received Surgery	Switched to Medicine
Died	27	2	15	6
Survived 2 yrs	296	48	354	20
Totals	323	50	369	26

Analysis	Medical	Surgery	z_{obs}	p-value
Intent to Treat	29/373 (7.8%)	21/395 (5.3%)	1.38	0.170
Efficacy	27/323 (8.4%)	15/369 (4.1 %)	2.37	0.018

12.2 Background and Review

Use an external reference to find the pdf, mean, and variance of a random variable that has a hyper geometric distribution. The population size $n = n_1 + n_2$, has n_1 (S)success' and n_2 (F)failures. The sample size is s. Let X be the number of successes in a sample of size s taken without replacement on this population, $x_1, x_2, ..., x_s$.

FDA evidence requires:

- Safety.
- Efficacy — how effective if a treatment is taken at regular dosage.
- Effectiveness — the highest level phase of a trial.

Example:
AABB (1)
ABAB (2)
BAAB (3)
BABA (4)
BBAA (5)
ABBA (6)
Block size = 4. Most imbalance is 2As, and 4Bs if trial stops early.

Example: Take the same sample, but with the block size = 6. Then, $\frac{6!}{3!3!} = 20$ cases.

Example: Take AAAABB. Then, there are $\frac{6!}{4!2!} = 15$ cases.

The time at which each subject is randomized is a defining moment in the conduct of a clinical trial. The *survival time* is the studied outcome. Fifty or more subjects are needed in a clinical trial. Suppose n_1 and n_2 are fixed by the allocation ratio. The problem is to determine n. The sample size and power involve α, β, and γ_1. n is the number of subjects to be randomized (not the number of subjects to recruit before randomization). Some subjects are lost to followup. Some subjects are non-compliance patients (non-adherence or protocol deviations).

Let x_i be independent random variables and let $W = \sum a_i x_i + c$. Then, $E(W) = \sum a_i E(x_i) + c$, and $Var(W) = \sum a_i^2 Var(x_i)$. Let z have a standard normal distribution. Then z^2 has a chi-square distribution with 1 degree of freedom. Consider the Rao-Blackwell variance decomposition. Let the pair (x, y) have a bivariate distribution. Then $Var(y) = Var[E(y|x)] + E[Var(y|x)]$. Consider the univariate Cramer δ theorem (i.e. the δ-method). Suppose that $\sqrt{n}(x_n - \mu) \rightarrow N(0, \sigma_1^2)$. Let $g(x)$ be any function differentiable at $x = \mu$. Then $\sqrt{n}[g(x_n) - g(\mu)] \rightarrow N(0, \sigma_1^2)$ where $\sigma_1^2 = [g'(\mu)]^2\sigma^2$. That is, $g(x_n)$ has approximately a normal distribution with a mean $g(\mu)$ and variance $\frac{[g'(\mu)]^2\sigma^2}{n}$.

The multivariate δ Theorem. Let $\underline{x}_n' = (x_{1n}, x_{2n}, ..., x_{kn})$ be a k-dimensional vector of random variables such that $\sqrt{n}(\underline{x}_n - \underline{\mu}) \rightarrow N(0, \Sigma)$ where Σ is a $k \times k$ covariance matrix. Let $g(x)$ be a differentiable function at $\underline{x} = \underline{\mu}$. Then $\sqrt{n}[g(\underline{x}_n) - g(\underline{\mu})] \rightarrow N(0, \sigma^2)$ where $\sigma^2 = \underline{a}'\Sigma\underline{a}$,

12.3 Large Sample Tests

Consider any statistic S_n that has approximately, if n is large, a normal distribution. Let H_0 and H_1 denote the null and alternative hypotheses. Use the notation:

Notation	Interpretation
$\mu = E(S_n)$	General expected value of S_n.
μ_0	Null expected value of S_n.
$\mu_1 = E_{h_1}(S_n)$	Expected value of S_n computed under the assumption that a particular H_1 is true.
$\sigma_{on}^2 = Var_{H_0}(S_n)$	Null variance of S_n.
$\sigma_{1H}^2 = Var_{H_1}(S_n)$	Variance of S_n computed under the assumption that a particular H_1 is true.
$\delta = \mu_1 - \mu_0$	Difference is expected values of S_n under H_0 and H_1.

Note that $\mu_0 = 0$. There are three cases:

1. Right sided alternatives: $H_0 : \mu \leq \mu_0$. $H_1 : \mu > \mu_0$. $\alpha =$ P(making a Type I error). The test statistic is $z = \frac{S_n - \mu_0}{\hat{\sigma}_{0n}}$ Reject H_0 if $z_{\text{observed}} \geq z_\alpha$.

2. Left sided alternatives: $H_0 : \mu \geq \mu_0$. $H_1 : \mu < \mu_0$. The test statistic is $z = \frac{S_n - \mu_0}{\hat{\sigma}_{0n}}$ Reject H_0 if $z_{\text{observed}} \leq z_\alpha$.

3. Two-sided alternatives: $H_0 : \mu = \mu_0$. $H_1 : \mu \neq \mu_0$. $\alpha =$ P(making a Type I error). The test statistic is $z = \frac{S_n - \mu_0}{\hat{\sigma}_{0n}}$ Reject H_0 if $z_{\text{observed}} \leq z_{\alpha/2}$ or if $z_{\text{observed}} \geq z_{\alpha/2}$

The sample size n needed so a two-sided test with significance level of α has the power $1 - \beta$ at a particular alternative μ_1(or $\delta_1 = \mu_1 - \mu_0$) must satisfy the following equation: $|\delta_1| = z_{\alpha/2}\sigma_{0n} + z_\beta\sigma_{1n}$ is called the *sample size power equation.*

Notes:

1. For a one-sided test, $\frac{\alpha}{2}$ must be replaced by α.

2. The power is greater than 0.50 iff $z_\beta > 0$.

The proof for two-sided alternatives: $H_0 : \mu = \mu_0$. $H_1 : \mu \neq \mu_0$. Reject H_0 if $z_{\text{obs}} \leq -z_{\alpha/2}$ or if $z_{\text{obs}} \geq z_{\alpha/2}$ or if $\frac{S_n - \mu_0}{\sigma_{0n}} \leq -z_{\alpha/2}$ or $\frac{S_n - \mu_0}{\sigma_{0n}} > z_{\alpha/2}$ Equivalently, reject H_0 if $S_n \leq \mu_0 - z_{\alpha/2}\sigma_{0n}$ or $S_n \geq \mu_0 + z_{\alpha/2}\sigma_{0n}$. The power at μ_1 is

$$P(\text{reject } H_0 | \ H_1 \text{ is true or } \mu = \mu_1) = P_{\mu_1}(S_n \leq \mu_0 - z_{\alpha/2}\sigma_{0n} \text{ or } z_n \geq \mu_o + z_{\alpha/2}\sigma_{0n}) =$$

$$P_{\mu_1}(S_n \leq \mu_0 - z_{\alpha/2}\sigma_{0n}) + P_{\mu_1}(S_n \geq \mu_0 + z_{\alpha/2}\sigma_{0n}) = P_{\mu_1}\left(\frac{S_n - \mu_1}{\sigma_{1n}} \leq \frac{\mu_0 - \mu_1 - z_{\alpha/2}\sigma_{0n}}{\sigma_{1n}}\right),$$

$$1 - \beta = P\left(z \leq \frac{\mu_0 - \mu_1 - z_{\alpha/2}\sigma_{0n}}{\sigma_{1n}}\right) + P\left(z \leq \frac{\mu_0 - \mu_1 + z_{\alpha/2}\sigma_{0n}}{\sigma_{1n}}\right) = P(z \leq a - c) + P(z \geq a + c)$$

where $a = \frac{\mu_0 - \mu_1}{\sigma_{1n}}$, and $c = \frac{z_{\alpha/2}\sigma_{0n}}{\sigma_{1n}}$,

- CASE 1: $a > 0$. If $a > 0$, then $P(z > a+c) \approx 0$. Choose $z_\beta > 0$. Then, $a - c = z_\beta = \frac{\mu_0 - \mu_1}{\sigma_{1n}} - \frac{z_{\alpha/2}\sigma_{0n}}{\sigma_{1n}} = z_\beta$, $\frac{\mu_0 - \mu_1}{\sigma_{1n}} = z_\beta + \frac{z_{\alpha/2}\sigma_{0n}}{\sigma_{1n}}$, $\mu_0 - \mu_1 = z_\beta\sigma_{1n} + z_{\alpha/2}\sigma_{0n}$, $|\mu_0 - \mu_1| = z_\beta\sigma_{1n} + z_{\alpha/2}\sigma_{0n}$, which is $|\delta_1|$.

- CASE 2: $a < 0$. $a < 0 \Rightarrow P(z < a - c) \approx 0$. So, the power $P(\mu_1) = P(z > a+c) = 1 - \beta$, $\Rightarrow a + c = -z_\beta$, $\frac{\mu_0 - \mu_1}{\sigma_{1n}} + \frac{z_{\alpha/2}\sigma_{0n}}{\sigma_{1n}} = -z_\beta$, $\frac{\mu_0 - \mu_1}{\sigma_{1n}} = -z_\beta - \frac{z_{\alpha/2}\sigma_{0n}}{\sigma_{1n}} = \mu_0 - \mu_1 = -z_\beta\sigma_{1n} - z_{\alpha/2}\sigma_{0n} - (\mu_0 - \mu_1) = z_\beta\sigma_{1n} + z_{\alpha/2}\sigma_{0n} = |\mu_0 - \mu_1| = z_\beta\sigma_{1n} + z_{\alpha/2}\sigma_{0n}$.

12.4 General Approach to Sample Size Determination

A parameter δ is chosen to represent the contrast between responses on the two treatments. Testing $\delta = 0$ under the null hypothesis H_0 tests for no difference. A significance level (usually 2-sided) of H_0 will be based on some statistic S_n, and a significance level of α. The sample size is $n = n_1 + n_2$ is chosen to ensure that the test has a specified power of $1 - \beta$ for a specified alternative δ_1. Allowance must be made for a hypothetical rate at which patients are lost to follow-up. Advantages of the sample size calculations include:

- They make investigators aware of the consequences of their choice of trial size.
- They may prevent implementing trials that are too small to be of any real value.

Difficulties with the sample size calculations include:

- The choices of α and β are somewhat arbitrary (though usually $\alpha = 0.05$ and $\beta \leq 0.10$) and different choices of α and β affect the value of n.
- The alternative δ_1 statistic is difficult to interpret. It may represent any of the following: a) the smallest clinically worth while difference, b) a difference worth detecting, and c) a difference thought likely to occur. Thus the value δ_1 must be chosen subjectively and agreement between investigators may not be easy to achieve.
- The sample size usually depends on other parameters (e.g. response rate in the control group and variance) about which there is some uncertainty.
- Information concerning the last difficulty listed can be obtained from: a) a pilot trial, b) an earlier Phase I or II study, and c) the literature concerning a similar study.

Conclusions: The sample size calculations should be regarded in a flexible way as providing guidance concerning the size of a study rather than a rigid prescription. They are a required part of the study protocol.

12.4.1 Sample Size and Power Calculations

Example 1: Suppose a trial is to be conducted to study the effectiveness of a new cholesterol lowering drug. The difference in serum cholesterol at baseline and six months after randomization is to be observed for each subject.

Group	Sample Size	Mean Change in Cholesterol Level	Sample Mean Difference	Variance
1 (drug)	n_1	v_1	$\bar{x}_1$	σ^2
2 (placebo)	n_2	v_2	$\bar{x}_2$	σ^2

Assume that subjects are allocated equally to the two groups. The hypotheses are $H_0 : v_1 = v_2$, versus $H_1 : v_1 > v_2$.

1. Determine $n = n_1 + n_2$ so that a 5% confidence level test has a power of 0.90 for detecting the difference $\delta = v_1 - v_2 = 10$ when $\bar{v} = 20$.
2. Determine the power of the 5% test at $\delta = 10$ if only $n = 100$ patients are recruited.
3. What power is attained if only $n = 36$ subjects are recruited?
4. What difference δ can be detected with a power of 0.90 and $n = 100$?
5. What sample size n is needed to detect the difference $\delta = 10$ with a power of 0.90 when using a two-tailed test with $\alpha = 0.05$?

Example 2: A trial is to be conducted to study two different ways of administering chemotherapy as a treatment for small cell lung cancer.

Treatment	Sample Size	Success
1 (new)	n_1	p_1
2 (control)	n_2	p_2

Previous studies indicate that the success rate for treatment 2 is $p_2 = 0.15$. Determine the total number n of participants that must be randomized so that a 5% level test of $H_0 : p_1 = p_2$ versus $H_1 : p_1 > p_2$ has a power of 0.90 for detecting an increase $\delta = p_1 - p_2$ of $\delta = 0.20$.

Example 3: Consider a repeated measures trial for comparing slopes (text book, page 113). The assumptions are

1. In the control group, the response variable decreases at a rate of 80 units per year ($\theta_1 = 80$).
2. A 25% reduction in this rate is expected for a new treatment (i.e. $\theta_2 = 60$).
3. Other studies indicate $\sigma_\epsilon = 150$ and $\sigma_\theta = 63$.
4. Subjects are to be allocated equally to the two treatment groups.

Determine $n = n_1 + n_2$ so that a 5% level test of $\delta = 0$ versus $H_1 : \delta \neq 0$ where $\delta = \theta_1 - \theta_2$ has a power of 0.90 for the following cases:

1. A 3 year study with 4 visits per year. $D = 3, k = 13$, one visit at baseline.
2. A 4 year study with 4 visits per year. $D = 4, k = 17$.

Example 4: This example can be found in the text book on page 108. Consider an eye study in which one eye is treated by laser surgery and the other eye by a standard therapy. The left and right eyes are randomly allocated to the two treatments. For each subject the data consists of two responses.

1. Vision improves (success) or does not improve (failure) in the eye receiving treatment 1.
2. Vision improves or does not improve in the eye receiving treatment 2.

π_i is the success rate for treatment $i = 1, 2$. $\pi_1 = 0.80, \pi_2 = 0.60, \delta = \pi_1 - \pi_2$. The discordant rate f is $f = 0.50$. Determine n so that a 5% level, two-sided test of $H_0 : \delta = 0$ versus $H_1 : \delta \neq 0$ has a power of 0.90 against the alternative $\delta = 0.20$.

12.5 General Sample Size and the Power Equation

$|\delta| = z_{\alpha/2}\sigma_{0n} + z_\beta \sigma_{1n}$. Comparing proportions with independent samples gives the following table:

Group	Sample Size	Population Proportion	Sample Proportion
1	n_1	p_1	$\widehat{p}_1$
2	n_2	p_2	$\widehat{p}_2$

$S_n = \widehat{p}_1 - \widehat{p}_2$, $\mu = E(S_n) = p_1 - p_2$, $\sigma_n^2 = Var(S_n) = \frac{p_1(1-p_1)}{n_1} + \frac{p_2(1-p_2)}{n_2}$, $H_0 : p_1 - p_2 = 0$. $H_1 : p_1 - p_2 > 0$. $\mu_0 = E_{H_0}(S_n) = 0$, $\mu_1 = E_{H_1}(S_n) = p_1 - p_2$, $\delta = \mu_1 - \mu_0 = p_1 - p_2$, $\sigma_{0n}^2 = Var_{H_0}(S_n) = \bar{p}(1-\bar{p})\left(\frac{1}{n_1} + \frac{1}{n_2}\right)$ $\sigma_{1n}^2 = Var_{H_1}(S_n) = \frac{p_1(1-p_1)}{n_1} + \frac{p_2(1-p_2)}{n_2}$ where $\bar{p} = \frac{p_1+p_2}{2}$ The sample size of the power equation is

$$|\delta| = z_\alpha \sigma_{0n} + z_\beta \sigma_{1n} = |\delta| = z_\alpha \sqrt{\bar{p}(1-\bar{p})}\sqrt{\left(\frac{1}{n_1} + \frac{1}{n_2}\right)} + z_\beta \sqrt{\frac{p_1(1-p_1)}{n_1} + \frac{p_2(1-p_2)}{n_2}}$$

Substitute $Q_i = \frac{n_i}{n}$ or $n_i = Q_i n$, for $i = 1, 2$. Then,

$$|\delta| = \frac{z_\alpha \sqrt{\bar{p}(1-\bar{p})}\sqrt{\frac{1}{Q_1} + \frac{1}{Q_2}} + z_\beta \sqrt{\frac{p_1(1-p_1)}{Q_1} + \frac{p_2(1-p_2)}{Q_2}}}{\sqrt{n}}.$$

$$z = \frac{\text{statistic} - E(\text{statistic})}{\text{std deviation}},$$

$$E(z) = \frac{1}{\sigma}x + \left(-\frac{\mu}{\sigma}\right) = \frac{1}{\sigma}E(x) + \left(-\frac{\mu}{\sigma}\right) = \frac{\mu}{\sigma} - \frac{\mu}{\sigma} = 0, \ \ Var(z) = \left(\frac{1}{\sigma}\right)^2 Var(x) = \frac{1}{\sigma^2}\sigma^2 = 1.$$

$$\widehat{p} = \frac{y}{n} = \frac{1}{n}y, \ \ E(\widehat{p}) = \frac{1}{n}E(y) = \frac{1}{n}np = p, \ \ Var(\widehat{p}) = \left(\frac{1}{n}\right)^2 Var(y) = \frac{1}{n^2}np(1-p) = \frac{p(1-p)}{n},$$

$$z = \frac{\widehat{p} - p}{\sqrt{\frac{p(1-p)}{n}}}, \ \ z' = \frac{\widehat{p} - p}{\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}}$$

Note that $\widehat{p} =$ sample mean

$$\mu = E(x) = 0(1-p) + 1p = p, \ \ \sigma^2 = E(x^2) - [E(x)]^2, \ \ E(x^2) = 0^2(1-p) + 1^2 p = p$$

$$\Rightarrow \sigma^2 = p - p^2 = p(1-p), \ \ Var(\widehat{p}) = \frac{p(1-p)}{n}$$

Suppose that $\bar{x}_1$, and $\bar{x}_2$ are independent.

$$S_n = \bar{x}_1 - \bar{x}_2 = (1)\bar{x}_1 + (-1)\bar{x}_2, \;\; E(S_n) = 1E(\bar{x}_1) + (-1)E(\bar{x}_x) = 1\mu_1 + (-1)\mu_2 = \mu_1 - \mu_2,$$

$$z = \frac{\bar{x}_1 - \bar{x}_2 - (\mu_1 - \mu_2)}{\sqrt{\frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}}}, \;\; z' = \frac{\bar{x}_1 - \bar{x}_2 - (\mu_1 - \mu_2)}{\sqrt{\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}}}, \;\; \widehat{p} = \frac{n_1\widehat{p}_1 + n_2\widehat{p}_2}{n_1 + n_2} = \frac{y_1 + y_2}{n_1 + n_2}.$$

The Q_i's are the allocation amounts. $Q_i = \frac{n_i}{n}$.

Example:

$$z = \frac{\widehat{p}_1 - \widehat{p}_2 - 0}{\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n_1} + \frac{\widehat{p}(1-\widehat{p})}{n_2}}}$$

Reject H_0 if $z_{\text{obs}} \geq z_\alpha = 1.645$. $p_2 = 0.15$. $\delta = p_1 - p_2 = p_1 - 0.15 \Rightarrow p_1 = 0.35$, because $\delta = 0.20$. The power is $1 - \beta = 0.90 \Rightarrow \beta = 0.10$, $z_{0.10} = 1.28; Q_1 = 0.60; Q_2 = 0.40$; $\bar{p} = \frac{p_1+p_2}{2} = \frac{0.15+0.35}{2} = 0.25$. Then, $0.20 = \frac{1.645\sqrt{0.25(0.75)}\sqrt{\frac{1}{0.60}+\frac{1}{0.40}}+1.28\sqrt{\frac{0.35(0.65)}{0.60}+\frac{0.15(0.85)}{0.40}}}{\sqrt{n}}$ Then, $\sqrt{n} = \frac{1.645\sqrt{0.25(0.75)}\sqrt{\frac{1}{0.60}+\frac{1}{0.40}}+1.28\sqrt{\frac{0.35(0.65)}{0.60}+\frac{0.15(0.85)}{0.40}}}{0.20} = 12.62$, $n = 159.2 \Rightarrow n = 160, n_1 = Q_1 n = 0.60(160) = 96, n_2 = Q_2 n = 0.40(160) = 64$. What about the non-compliance people? Reference page 107 of the text book.

Definition: A *drop-out* is any participant randomized to the treatment group who does not adhere to the assigned treatment or treatment schedule. A *drop-in* is any participant randomized to the control group who begins to use the study treatment. The text book, page 108, uses the following notation: R_0 = drop-out rate, and R_I = drop-in rate. n = unadjusted sample size, n^* = adjusted sample size = $\frac{n}{(1-R_0-R_I)^2}$.

Example: Suppose $R_0 = 0.20, R_I = 0.05$, and $n = 200$. Then, $n^* = \frac{200}{(1-0.20-0.05)^2} = \frac{200}{(0.75)^2} = 356$. Another example appears on page 108 of the text book using p_I^*, p_C^* from p_I, and p_C.

12.5.1 Further Background

In all that follows we will primarily use the following:

1. Let X be any random variable and let a, b be any constants. Then, $E(ax + b) = aE(x) + b$ and $Var(ax + b) = a^2 Var(x)$.
2. The standardized form of any random variable X is $z = \frac{x-\mu}{\sigma}$. As a consequence of (1), any standardized random variable z has mean, $E(z) = 0$, and $Var(z) = 1$.
3. Let $x_1, x_2, ..., x_n$ be any independent random variables and let $a_1, a_2, ..., a_n$ be any constants. Then,
$$E\left(\sum_{i=1}^{n} a_i x_i\right) \sum_{i=1}^{n} a_i E(x_i), \;\; Var\left(\sum_{i=1}^{n} a_i x_i\right) \sum_{i=1}^{n} a_i^2 Var(x_i),$$
4. An important special case of (3) is $E(a_1x_1 + a_2x_2) = a_1E(x_1) + a_2E(x_2)$, and $Var(a_1x_1 + a_2x_2) = a_1^2 Var(x_1) + a_2^2 Var(x_2)$.

Random Sample from a Single Population

Let $x_1, x_2, ..., x_n$ be iid random variables with mean μ and variance σ^2. That is, $E(x_i) = \mu$, and $Var(x_i) = \sigma^2$. The sample mean $\bar{x}$ is a linear function of independent random variables. $\bar{x} = \frac{x_1+x_2+\cdots+x_n}{n}$. Using (3), we have

$$E(\bar{x}) = \frac{1}{n}E(x_1) + \frac{1}{n}E(x_2) + \cdots + \frac{1}{n}E(x_n) = \frac{1}{n}\mu + \frac{1}{n}\mu + \cdots + \frac{1}{n}\mu = n\left(\frac{1}{n}\mu\right) = \mu.$$

$$Var(\bar{x}) = \left(\frac{1}{n}\right)^2 Var(x_1) + \left(\frac{1}{n}\right)^2 Var(x_2) + \cdots + \left(\frac{1}{n}\right)^2 Var(x_n) = \frac{1}{n^2}\sigma^2 + \frac{1}{n^2}\sigma^2 + \cdots + \frac{1}{n^2}\sigma^2 =$$
$$n\left(\frac{\sigma^2}{n^2}\right) = \frac{\sigma^2}{n}.$$

Standardized Form of $\bar{X}$

Using (2) we write,

$$z = \frac{\bar{x} - E(\bar{x})}{\sqrt{Var(\bar{x})}}, \quad z = \frac{\bar{x} - \mu}{\sigma/\sqrt{n}}.$$

We know that z has a distribution with mean zero and variance 1.

Modified Standardized Form o $\bar{X}$

The standardized form of $\bar{x}$ can not be used for inference about a population mean μ unless the value of σ is known. Since usually the value of σ is not known, we replace σ by its estimator, namely, the sample standard deviation, $s = \sqrt{s^2}$. The result is the modified standardized form $z' = \frac{\bar{x}-\mu}{s/\sqrt{n}}$.

The Central Limit Theorem

The Central Limit Theorem implies that if n is large ($n > 30$) then both z and z' have approximately standard normal distributions. If $x_1, x_2, ..., x_n$ is a random sample from a normal distribution, then

a. z has exactly a standard normal distribution for every n.

b. z' has exactly a $t-$distribution for every n.

In case (b), the modified standardized form z' is usually labeled T to denote that it has a $t-$distribution. That is, we write $T = \frac{\bar{x}-\mu}{s/\sqrt{n}}$. since if the sample arises from a normal distribution, then T has a $t-$distribution with degrees of freedom $n-1$. In clinical trials the sample size is usually much larger than 30 so we use the normal approximation to the distribution of z'.

Special Case: Binary Response Variables

As before assume that we have iid random variables $x_1, x_2, ..., x_n$ where the response of each subject is binary:

$$x_i = \begin{cases} 1, & \text{if subject \# i responds favorably to treatment.} \\ 0, & \text{otherwise.} \end{cases}$$

It is clear that each x_i then has the following probability distribution:

x	0	1
$f(x)$	$1-p$	p

where $p = P(x_i = 1)$ is the probability that subject i responds favorable to treatment. Note that $x_1 + x_2 + \cdots + x_n$ is the total number of successes occurring in n iid trials, call it y. We know y has a binomial distribution with pdf

$$f(y) = \binom{n}{y} p^y (1-p)^{n-y}, y = 0, 1, 2, ..., n.$$

The mean and variance of a binomial random variable y are $E(y) = np$, and $Var(y) = np(1-p)$. We usually estimate the parameter p by the sample proportion $\widehat{p} = \frac{y}{n}$. At this point we should use (1) to get the mean, variance, and standardized form of $\widehat{p}$

Since iid binary random variables are a special case of general iid random variables, we should be able to apply earlier results obtained for the general case. In particular note that $\widehat{p} = \frac{y}{n} = \frac{x_1+x_2+\cdots+x_n}{n}$. Thus $\widehat{p}$ is actually a sample mean and we know that

$$\left.\begin{array}{l} E(\widehat{p}) = \mu \\ Var(\widehat{p}) = \frac{\sigma^2}{n} \end{array}\right\}$$

where μ is the population mean and σ^2 is the population variance. μ and σ^2 can be calculated from the pdf

x	0	1
$f(x)$	$1-p$	p

Independent Samples from 2 Populations

Population	Population Mean	Population Variance	Sample Size	Sample Mean	Sample Variance
#1	μ_1	σ_1^2	n_1	$\bar{x}_1$	s_1^2
#2	μ_2	σ_2^2	n_2	$\bar{x}_2$	s_2^2

Since the samples are take independently, $\bar{x}_1$ and $\bar{x}_2$ are independent random variables. Usually we want to estimate $\mu_1 - \mu_2$ and for this reason we are interested in the statistic $\bar{x}_1 - \bar{x}_2$. Note that $\bar{x}_1 - \bar{x}_2$ is a linear function of $\bar{x}_1$ and $\bar{x}_2$. That is $\bar{x}_1 - \bar{x}_2 = (1)\bar{x}_1 + (-1)\bar{x}_2$. Using our theorems on expected value and variance of linear functions of independent random variables, we have

$$E(\bar{x}_1 - \bar{x}_2) = (1)E(\bar{x}_1) + (-1)E(\bar{x}_2) = (1)\mu_1 + (-1)\mu_2 = \mu_1 - \mu_2.$$

$$Var(\bar{x}_1 - \bar{x}_2) = Var[(1)\bar{x}_1 + (-1)\bar{x}_2] = (1)^2 Var(\bar{x}_1) + (-1)^2 Var(\bar{x}_2) = \frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2}.$$

Let z and z' be the standardized form and the modified standardized forms of $\bar{x}_1 - \bar{x}_2$. The Central Limit Theorem implies that if n_1 and n_2 are large, both greater than 30, then z and z' have approximately standard normal distributions. Often we are willing to assume that the two populations have a common variance $\sigma^2 = \sigma_1^2 = \sigma_2^2$. Then the standardized form of $\bar{x}_1 - \bar{x}_2$ is

$$z = \frac{\bar{x}_1 - \bar{x}_2 - (\mu_1 - \mu_2)}{\sigma\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}}$$

Since the value of σ is usually unknown we estimate σ^2 by forming a weighted average of s_1^2 and s_2^2.

$$s_p = \frac{(n_1 - 1)s_1^2 + (n_2 - 1)s_2^2}{n_1 + n_2 - 2}$$

When the two populations can be assumed to have a common variance, the modified standardized form of $\bar{x}_1 - \bar{x}_2$ is

$$z = \frac{\bar{x}_1 - \bar{x}_2 - (\mu_1 - \mu_2)}{s_p\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}}$$

As before, the Central Limit Theorem implies that z' has approximately a standard normal distribution if $n_i \geq 30, i = 1, 2$. Alternatively, if the independent samples arise from normal distributions, then z' has exactly a $t-$distribution with $n_1 + n_2 - 2$ degrees of freedom and is usually labeled T rather than z'.

Independent Samples and a Binary Response

Population	Population Proportion	Sample Size	Number Giving a Favorable Response	Sample Proportion
#1	p_1	n_1	y_1	$\widehat{p}_1 = y_1/n_1$
#2	p_2	n_2	y_2	$\widehat{p}_2 = y_2/n_2$

Clearly $\widehat{p}_1 - \widehat{p}_2$ is the difference of two sample means. So this case is very similar to the one just described (except that there is no possibility that binary random variables can have normal distributions. So there is no $T-$statistic). Now determine the mean, variance and standardized form of $\widehat{p}_1 - \widehat{p}_2$.

$$E(\widehat{p}_1 - \widehat{p}_2) = E[(1)\widehat{p}_1 + (-1)\widehat{p}_2] = (1)E(\widehat{p}_1) + (-1)E(\widehat{p}_2) = p_1 - p_2.$$

$$Var(\widehat{p}_1 - \widehat{p}_2) = Var[(1)\widehat{p}_1 + (-1)\widehat{p}_2] = (1)^2 Var(\widehat{p}_1) + (-1)^2 Var(\widehat{p}_2) =$$

$$Var(\widehat{p}_1) + Var(\widehat{p}_2) = \frac{p_1(1-p_1)}{n_1} + \frac{p_2(1-p_2)}{n_2}.$$

The standardized form is

$$z = \frac{\widehat{p}_1 - \widehat{p}_2 - (p_1 - p_2)}{\sqrt{\frac{p_1(1-p_1)}{n_1} + \frac{p_2(1-p_2)}{n_2}}}$$

The modified standardized form is

$$z' = \frac{\widehat{p}_1 - \widehat{p}_2 - (p_1 - p_2)}{\sqrt{\frac{\widehat{p}_1(1-\widehat{p}_1)}{n_1} + \frac{\widehat{p}_2(1-\widehat{p}_2)}{n_2}}}$$

According to the Central Limit Theorem, z and z' have approximate standard normal distributions.

Confidence Limits for $p_1 - p_2$

To obtain $100(1-\alpha)\%$ confidence limits, choose the limit $z_{\alpha/2}$ from the tabled normal distribution so that

$$P\left(-z_{\alpha/2} < Z' < z_{\alpha/2}\right) = 1 - \alpha.$$

Then,

$$P\left(-z_{\alpha/2} < \frac{\widehat{p}_1 - \widehat{p}_2 - (p_1 - p_2)}{\sqrt{\frac{\widehat{p}_1(1-\widehat{p}_1)}{n_1} + \frac{\widehat{p}_2(1-\widehat{p}_2)}{n_2}}} < z_{\alpha/2}\right) = 1 - \alpha.$$

Algebraic manipulation gives $1 - \alpha =$

$$P\left(\widehat{p}_1 - \widehat{p}_2 - z_{\alpha/2}\sqrt{\frac{\widehat{p}_1(1-\widehat{p}_1)}{n_1} + \frac{\widehat{p}_2(1-\widehat{p}_2)}{n_2}} < p_1 - p_2 < \widehat{p}_1 - \widehat{p}_2 + z_{\alpha/2}\sqrt{\frac{\widehat{p}_1(1-\widehat{p}_1)}{n_1} + \frac{\widehat{p}_2(1-\widehat{p}_2)}{n_2}}\right)$$

Thus, the upper and lower confidence limits are

$$\widehat{p}_1 - \widehat{p}_2 \pm z_{\alpha/2}\sqrt{\frac{\widehat{p}_1(1-\widehat{p}_1)}{n_1} + \frac{\widehat{p}_2(1-\widehat{p}_2)}{n_2}}$$

Testing the Hypothesis

The standardized form under H_0 is

$$z = \frac{\widehat{p}_1 - \widehat{p}_2 - 0}{\sqrt{\frac{p_1(1-p_1)}{n_1} + \frac{p_2(1-p_2)}{n_2}}}$$

and the modified standardized form under H_0 is

$$z' = \frac{\widehat{p}_1 - \widehat{p}_2 - 0}{\sqrt{\frac{\widehat{p}_1(1-\widehat{p}_1)}{n_1} + \frac{\widehat{p}_2(1-\widehat{p}_2)}{n_2}}}$$

which is the proper test statistic.

12.6 Comparing Slopes with Repeated Measures

A trial is sometimes designed to investigate changes over time in some characteristic that is measured repeatedly for each subject. The characteristic may be blood pressure, bone mass, cholesterol level, lung volume, etc. A model sometimes used in this setting is the simple linear random effects model with follow-up time being an explanatory variable. The model is similar to the ordinary straight line model except that the slope and intercept are permitted to vary between different subjects. Thus, the slope and intercept are modeled as random quantities and, for this reason, the model is called a *linear random effects model.*

Let k be the number of planned follow-up visits and $x_1, x_2, ..., x_k$ be the follow-up times measured from the date of randomization. In the Linear Random Effects model, y_{ij} is response of subject i at follow-up time $x_j : y_{ij} = \gamma_i + \theta_i x_j + \epsilon_{ij}, i = 1, 2, ..., n; j = 1, 2, ..., k$, where γ_i is the subject specific intercept, θ_i is the subject specific slope, and ϵ_{ij} is the random error term. The model assumptions are:

1. (γ_i, θ_i) are iid random vectors that have a bivariate normal distribution with mean vector (γ, θ) and covariance matrix, $Var(\gamma_i) = \sigma_\gamma^2, Var(\theta_i) = \sigma_\theta^2$, and $Cov(\gamma, \theta_i) = \sigma_{\gamma\theta}$.
2. ϵ_{ij} are iid and have a normal distribution with mean zero and variance σ_ϵ^2.
3. (γ_i, θ_i) and ϵ_{ij} are independent collections of random variables.

Note: The model implies that

1. Repeated observations on the same subject are dependent random variables.
2. Observations on different subjects are independent.

12.6.1 Estimators of Subject Specific Slopes

Let L_i be the number of visits completed by subject i. We assume there are no missed interim visits but that subject i may not complete all k visits. Thus, $L_i = k$ only if subject i completes all k visits. The data for subject i are $(x_j, y_{ij}), j = 1, 2, 3, ..., L_i; i = 1, 2, ..., n$. The least squares estimator of the subject specific slope θ_i is $\widehat{\theta}_i = \sum_{j=1}^{L_i} \frac{(x_j - \bar{x}_i)y_{ij}}{S_i}$, where $S_i = \sum_{j=1}^{L_i}(x_j - \bar{x}_i)^2$, and $\bar{x}_i = \frac{x_1 + x_2 + \cdots + \bar{x}_{L_i}}{L_i}$.

Expected Value and Variance of Slope Estimator for a Single Subject

Standard results for the straight line regression model with fixed slope and intercept give the following: $E(\widehat{\theta}_i|\theta_i) = \theta_i \; Var(\widehat{\theta}_i|\theta_i) = \frac{\sigma_\epsilon^2}{S_i}$ To derive the unconditional mean and variance, recall that $E[E(Y|X)] = E(Y)$, and $Var(Y) = Var[E(Y|X)] + E(Var(Y|X)]$. Applying this to the two equations above gives: $E(\widehat{\theta}_i) = E(\theta_i) = \theta$, and

$$v_i = Var(\widehat{\theta}_i) = Var[E(\widehat{\theta}_i|\theta_i)] + E[Var(\widehat{\theta}_i|\theta_i)] = Var(\theta_i) + E\left[\frac{\sigma_\epsilon^2}{S_i}\right] = \sigma_\theta^2 + \frac{\sigma_\epsilon^2}{S_i} = \sigma_\theta^2[1 + R/S_i]$$

where $R = \frac{\sigma_\epsilon^2}{\sigma_\theta^2}$.

Estimate of the Population Mean Slope

Since observations on different subjects are assumed independent, we have, for n subjects, n different estimators of θ. Namely, $\widehat{\theta}_1, \widehat{\theta}_2, ..., \widehat{\theta}_n$ are all estimators of θ. How should we combine the subject specific slope estimators to get a single estimate of θ? The maximum likelihood estimator of θ is the following weighted linear combination of $\widehat{\theta}_1, \widehat{\theta}_2, ..., \widehat{\theta}_n$. $\widehat{\theta} = \frac{\sum_{i=1}^n v_i^{-1}\widehat{\theta}_i}{\sum_{i=1}^n v_i^{-1}}$ where $v_i = \sigma_\theta^2[1 + R/S_i], i = 1, 2, ..., n$.

Expected Value and Variance of Slope Estimation

Note that $\widehat{\theta}$ is a linear function of $\widehat{\theta}_1, \widehat{\theta}_2, ..., \widehat{\theta}_n$. Thus,

$$E(\widehat{\theta}) = E\left[\frac{\sum_{i=1}^n v_i^{-1}\widehat{\theta}_i}{\sum_{i=1}^n v_i^{-1}}\right] = \frac{\sum_{i=1}^n v_i^{-1}E(\widehat{\theta}_i)}{\sum_{i=1}^n v_i^{-1}} = \theta\frac{\sum_{i=1}^n v_i^{-1}}{\sum_{i=1}^n v_i^{-1}} = \theta.$$

Since $\widehat{\theta}_1, \widehat{\theta}_2, ..., \widehat{\theta}_n$ are independent, we have

$$Var(\widehat{\theta}) = \frac{\sum_{i=1}^n (v_i^{-1})^2 Var(\widehat{\theta}_i)}{\left(\sum_{=1}^n v_i^{-1}\right)^2}, \ \ (v_i^{-1})^2 Var(\widehat{\theta}_i) = \frac{1}{v_i^2}Var(\widehat{\theta}_i) = \frac{1}{v_i},$$

since by definition $v_i = Var(\widehat{\theta}_i)$. Thus,

$$Var(\widehat{\theta}) = \frac{\sum_{i=1}^n v_i^{-1}}{\left(\sum_{i=1}^n v_i^{-1}\right)^2} = \frac{1}{\sum_{i=1}^n v_i^{-1}}$$

Comparing Slopes for Two Treatment Groups

Group	Population Mean Slope	Sample Size
1	θ_1	n_1
2	θ_2	n_2

Some other notation: L_{1i} is the number of visits completed by subject i in group 1. L_{2i} is the number of visits completed by subject i in group 2.

$$S_{1i} = \sum_{j=1}^{L_{1i}}(x_j - \bar{x}_{1i})^2, \ \ S_{2i} = \sum_{j=1}^{L_{2i}}(x_j - \bar{x}_{2i})^2.$$

The parameters $\sigma_\theta^2, \sigma_\gamma^2, \sigma_{\theta\gamma}, \sigma_\epsilon^2$ are assumed to be identical for the two groups. $\widehat{\theta}_1$ is the slope estimator for group 1. $\widehat{\theta}_2$ is the slope estimator for group 2. Observations in the two groups are assumed to be independent. Thus, $\widehat{\theta}_1$ and $\widehat{\theta}_2$ are independent random variables.

Mean and Variance of the Standardized form of $\widehat{\theta}_1 - \widehat{\theta}_2$

$$E[\widehat{\theta}_1 - \widehat{\theta}_2] = E(\widehat{\theta}_1) - E(\widehat{\theta}_2) = \theta_1 - \theta_2.$$

$$Var(\widehat{\theta}_1 - \widehat{\theta}_2) = (1)^2 Var(\widehat{\theta}_1) + (-1)^2 Var(\widehat{\theta}_2) = Var(\widehat{\theta}_1) + Var(\widehat{\theta}_2) = \left(\sum_{i=1}^{n_1} v_{1i}^{-1}\right)^{-1} + \left(\sum_{i=1}^{n_2} v_{2i}^{-1}\right)^{-1}$$

where $v_{1i} = \sigma_\theta^2[1 + R/S_{1i}]$, and $v_{1i} = \sigma_\theta^2[1 + R/S_{2i}]$

Standardized Form of $\widehat{\theta}_1 - \widehat{\theta}_2$

$$Z = \frac{\widehat{\theta}_1 - \widehat{\theta}_2 - (\theta_1 - \theta_2)}{\sqrt{\left(\sum_{i=1}^{n_1} v_{1i}^{-1}\right)^{-1} + \left(\sum_{i=1}^{n_2} v_{2i}^{-1}\right)^{-1}}}$$

Sample Size and Power (Ideal Conditions)

We assume that each subject will complete all follow-up visits. Then, $L_{1i} = L_{2i} = k$, and

$$S_{1i} = S_{2i} = \sum_{j=1}^{k} (x_j - \bar{x})^2.$$

Let

$$S = \sum_{j=1}^{k} (x_j - \bar{x})^2.$$

Then, $v_{1i} = v_{2i} = \sigma_\theta^2[1 + R/S]$. We have $\delta = \theta_1 - \theta_2$.

$$Var(\widehat{\theta}_1 - \widehat{\theta}_2) = \left(\sum_{i=1}^{n_1} v_{1i}^{-1} \right)^{-1} + \left(\sum_{i=1}^{n_2} v_{2i}^{-1} \right)^{-1} = \sigma_\theta^2[1 + R/S] \left[\frac{1}{n_1} + \frac{1}{n_2} \right].$$

Sample Size — Power Equation

The hypotheses are $H_0 : \delta = 0$ versus $H_1 : \delta > 0$, where $\delta = \theta_1 - \theta_2$, and $\widehat{\delta} = \widehat{\theta}_1 - \widehat{\theta}_2$. $\mu_1 = E_{H_1}(\widehat{\delta}) = \delta_1$, $\mu_0 = E_{H_0}(\widehat{\delta}) = 0$.

$$\sigma_{0n}^2 = \sigma_{1n}^2 = Var(\widehat{\theta}_1 - \widehat{\theta}_2) = \sigma_\theta^2[1 + R/S] \left[\frac{1}{n_1} + \frac{1}{n_2} \right] = \frac{\sigma_\theta^2[1 + R/S]}{n} \left[\frac{1}{Q_1} + \frac{1}{Q_2} \right].$$

$$|\mu_1 - \mu_0| = z_\alpha \sigma_{0n} + z_\beta \sigma_{1n}$$

or

$$|\delta_1| = \frac{(z_\alpha + z_\beta)\sigma_\theta \sqrt{1 + R/S} \sqrt{\frac{1}{Q_1} + \frac{1}{Q_2}}}{\sqrt{n}}$$

$$n = \frac{(z_\alpha + z_\beta)^2 \sigma_\theta^2 (1 + R/S) \left[\frac{1}{Q_1} + \frac{1}{Q_2} \right]}{(\delta_1)^2}$$

A Simple Formula for S

It is common to make simplifying assumptions when determining sample size. We assume the follow-up times are equally spaced but may begin at an arbitrary point in time. That is, $x_1 = b, x_2 = b + a, x_3 = b + 2a, ..., x_k = b + (k-1)a$. Since $S = \sum_{i=1}^{k} (x_i - \bar{x})^2$ does not depend on b, we can set b equal to any convenient value to get a simple form of S. Let $b = a$. Then, $x_i = ai, i = 1, 2, ..., k$ and

$$\sum_{i=1}^{k} x_i = a \sum_{i=1}^{k} i = \frac{ak(k+1)}{2}, \quad \sum_{i=1}^{k} x_i^2 = a^2 \sum_{i=1}^{k} i^2 = \frac{a^2 k(k+1)(2k+1)}{6}.$$

Thus,

$$S = \sum_{i=1}^{2} x_i^2 - \frac{\left(\sum_{i=1}^{k} x_i \right)^2}{k} = \frac{a^2 k(k+1)(2k+1)}{6} - \frac{a^2 k(k+1)}{4} = \frac{a^2 k(k^2 - 1)}{12}.$$

Let D equal the duration of the follow-up. $D = x_k - x_1 = ka - a = a(k-1)$. Then,

$$S = \frac{a^2 k(k-1)^2(k+1)}{12(k-1)} = \frac{D^2 k(k+1)}{12(k-1)}.$$

Our sample size formula becomes

$$n = \frac{(z_\alpha + z_\beta)^2 \sigma_\theta^2 (1 + R/S)\left[\frac{1}{Q_1} + \frac{1}{Q_2}\right]}{(\delta_1)^2} = \frac{(z_\alpha + z_\beta)^2 \sigma_\theta^2 \left[1 + \frac{12R(k-1)}{D^2 k(k+1)}\right]}{(\delta_1)^2}.$$

The choice of k and D depend on:

(a) How long we can afford to follow participants.

(b) How many times a participant may be willing to visit a clinic.

Example: Text book, page 113. Assumptions:

1. In the control group, the response variable decreases at a rate of 80 units per year (i.e. $\theta_1 = 80$).
2. A 25% reduction in this rate is expected in the treatment group ($\theta_2 = 60$).
3. Other studies indicate that $\sigma_\epsilon = 150$ and $\sigma_\theta = 63$.
4. Equal allocation: $Q_1 = Q_2 = \frac{1}{2}$.

Determine the sample size n needed so a 5% level test has a power of 0.90 for

a. a 3 year study with 4 visits per year (i.e. $D = 3, k = 13$, one visit is baseline).

b. a 4 year study with 4 visits per year (i.e. $D = 4, k = 17$).

Note that $k \geq 2$ due to slope calculations. The solution is as follow: $H_0 : \delta = 0$, $H_A \delta \neq 0$. $\sigma_\epsilon = 150$, $\sigma_\theta = 63$, $R = \frac{\sigma_\epsilon}{\sigma_\theta}^2 = 5.67$, Let $\alpha = 0.05$. Then $z_{\alpha/2} = 1.96$. If power is set at 0.90, Then $Z_{2,3} = 1.28$. $\delta_1 = \theta_1 - \theta_2 = 80 - 60 = 20$.

1. $D = 3, k = 13$.

$$n = \frac{(z_{\alpha/2} + z_\beta)^2 \sigma^2}{\delta^2}\left[1 + \frac{12R(k-1)}{D^2 k(k+1)}\right]\left[\frac{1}{Q_1} + \frac{1}{Q_2}\right] = \frac{(1.96 + 1.28)^2 (63)^2}{(20)^2}\left[1 + \frac{12(5.67)(12)}{(3)^2(13)(14))}\right] = 625.$$

2. $D = 4$, $k = 17$.

$$n = \frac{(1.96 + 1.28)^2 (63)^2}{(20)^2}\left[1 + \frac{12(5.67)(16)}{(4)^2(17)(18))}\right] = 510.$$

12.6.2 Paired Binary Response

Occasionally, trials are conducted by using matched pairs of subjects or some form of natural pairing.

Example: Consider an eye study in which one eye is treated for loss of visual acuity by laser surgery and the other eye is treated by standard therapy. The left and right eyes are randomly allocated in the two treatments. For each subject, the data consists of two responses:

a. Vision improves (success) or does not improve (failure) in the eye receiving treatment 1.

b. Vision improves (success) or does not improve (failure) in the eye receiving treatment 2.

Main Parameters of Interest

Let π_i, $i = 1, 2$ denote the success rate for treatment $i = 1, 2$. Then the main parameter is $\delta = \pi_1 - \pi_2$ is the difference in success rates of the two treatments. In the following, we discuss the basis for McNemar's test for comparing π_1 and π_2. We then derive the sample size, the power equation. We will see that McNemar's test is in some ways similar to the paired $t-$test and in other ways similar to a test for comparing proportions with independent samples.

Notation

Let u_i be the response of subject i to treatment 1.

$$u_i = \begin{cases} 1, & \text{if success occurs on treatment 1} \\ 0, & \text{otherwise} \end{cases}$$

Let v_i be the response of subject i to treatment 2.

$$v_i = \begin{cases} 1, & \text{if success occurs on treatment 2} \\ 0, & \text{otherwise} \end{cases}$$

Assumptions

(u_i, v_i) are independent and identically distributed pairs with the following probability distribution:

(u,v)	(0,0)	(0,1)	(1,0)	(1,1)
$f(u, v)$	$\pi_{0,0}$	$\pi_{0,1}$	$\pi_{1,0}$	$\pi_{1,1}$

Recall that π_i is the success rate of treatment i. $\pi_1 = P(u = 1) = P(u = 1, v = 0) + P(u = 1, v = 1) = \pi_{1,0} + \pi_{1,1}$. Similarly, $\pi_2 = P(v = 1) = P(u = 0, v = 1) + P(u = 1, v = 1) = \pi_{0,1} + \pi_{1,1}$. Note that $\delta = \pi_1 - \pi_2 = (\pi_{1,0} - \pi_{1,1}) - (\pi_{0,1} - \pi_{1,1}) = \pi_{1,0} - \pi_{0,1}$. The outcomes (0,1) and (1,0) are called *discordant responses.* Thus, δ is the difference in success rates which is the same as the difference in discordant response rate.

Analysis Based on Within Subject Differences

Let $w_i = u_i - v_i$, $i = 1, 2, ..., n$. The w_i are iid with the following probability distribution:

w	-1	0	1
$g(w)$	$\pi_{0,1}$	$(\pi_{0,0} + \pi_{1,1})$	$\pi_{1,0}$

That is, $g(-1) = P(w = -1) = P(u - v = -1) = P(u = 0 \text{ and } v = 1) = \pi_{0,1}$. $g(0) = P(w = 0) = P(u - v = 0) = P(u = 0 \text{ and } v = 0) + P(u = 1 \text{ and } v = 1) = \pi_{0,0} + \pi_{1,1}$. Similarly, $g(1) = \pi_{1,0}$. $E(w_i) = -1(\pi_{0,1}) + 0(\pi_{0,0} + \pi_{1,1}) + 1(\pi_{1,0}) = \pi_{1,0} - \pi_{0,1} = \delta$. $Var(w_i) = E(w_i^2) - [E(w_i)]^2$, $E(w_i^2) = (-1)^2\pi_{0,1} + (0)^2(\pi_{0,0} - \pi_{1,1}) + (1)^2\pi_{1,0} = \pi_{1,0} + \pi_{0,1}$. $Var(w_i) = (\pi_{1,0} + \pi_{0,1}) - \delta^2 = f - \delta^2$ where $f = \pi_{1,0} + \pi_{0,1}$ is the discordant response rate. Let $\bar{w} = \sum_{i=1}^{n} \frac{w_i}{n}$. Then $E(\bar{w}) = \delta$ and $Var(w_i) = \frac{f-\delta^2}{n}$. For large n, the following quantity has approximately a standard normal distribution: $Z = \frac{\bar{w}-\delta}{\sqrt{\frac{f-\delta^2}{n}}}$.

An Alternative For of $\bar{w}$

Let $Y_{i,j}$ be the number of subjects for which the response is the pair (i, j). $(i, i) = (0, 0), (0, 1), (1, 0), (1, 1)$. Then $(Y_{0,0}, Y_{1,0}, Y_{0,1}, Y_{1,1})$ has a multinomial distribution and each $Y_{i,j}$ has a marginal binomial distribution $\sum_{i,j} Y_{i,j} = n$. $\pi_{i,j}$ is the sample proportion of the subjects giving response $(i, j) = \frac{Y_{i,j}}{n}$. To relate these quantities to $\bar{w}$, note that $\sum_{i=1}^{n} u_i$ is the number of successes in treatment 1 which is $Y_{1,0}+Y_{1,1}$. $\sum_{i=1}^{n}\frac{u_i}{n} = \frac{Y_{1,0}+Y_{1,1}}{n} = \hat{\pi}_{1,0}+\hat{\pi}_{1,1}$ Similarly, $\sum_{i=1}^{n} v_i$ is the number of successes in treatment 2 which is $Y_{0,1}+Y_{1,1}$. $\sum_{i=1}^{n}\frac{v_i}{n} = \frac{Y_{0,1}+Y_{1,1}}{n} = \hat{\pi}_{0,1}+\hat{\pi}_{1,1}$. Thus,

$$\bar{w} = \sum_{i=1}^{n}\frac{(u_i-v_i)}{n} = \frac{\sum_{i=1}^{n} u_i}{n} - \frac{\sum_{i=1}^{n} v_i}{n} = \hat{\pi}_1-\hat{\pi}_2 = (\hat{\pi}_{1,0}+\hat{\pi}_{1,1})-(\hat{\pi}_{0,1}+\hat{\pi}_{1,1}) = (\hat{\pi}_{1,0}-\hat{\pi}_{0,1})$$

which is the sample difference in discordant response rates.

McNemar's Test

Consider the hypothesis $H_0:\delta=0$ versus $H_A:\delta\neq 0$ where $\delta=\pi_1-\pi_2=\pi_{1,0}-\pi_{0,1}$. Let π denote the common value of $\pi_{1,0}$ and $\pi_{0,1}$. An estimate of π is $\bar{p}=\frac{1}{2}\left(\hat{\pi}_{1,0}+\hat{\pi}_{0,1}\right)$. $E_{H_0}(\bar{w})=\delta=0$. $Var_{H_0}(\bar{w})=\frac{f-\delta^2}{n}=\frac{2\pi}{n}$. with $\delta=0$ and $f=\pi_{1,0}+\pi_{0,1}=2\pi$. The test statistic is $Z=\frac{\bar{w}-0}{\sqrt{\frac{2\bar{p}}{n}}}$. This is equivalent to $Z=\frac{\hat{\pi}_1-\hat{\pi}_2}{\sqrt{\frac{2\bar{p}}{n}}}$. Z^2 is the McNemar's statistic, which has approximately a chi-square distribution with degrees of freedom equal to 1. Reject H_0 if $z_{\text{obs}}\leq -z_{\alpha/2}$ or if $z_{\text{obs}}\geq z_{\alpha/2}$ which is equivalent to, reject H_0 if $z^2\geq z_{\alpha}$.

Sample Size-Power Equation

Recall that $|\delta|=z_{\alpha/2}\sigma_{0n}+z_\beta\sigma_{1n}$ where $\delta=E(\bar{w})$ and $\sigma_{0n}^2=Var_{H_0}(\bar{w})=\frac{2\pi}{n}$ and $\sigma_{1n}^2=Var_{H_A}(\bar{w})=\frac{f-\delta^2}{n}$. Substituting gives, $|\delta|=z_{\alpha/2}\frac{\sqrt{2\pi}}{\sqrt{n}}+z_\beta\frac{\sqrt{f-\delta^2}}{\sqrt{n}}$ or $\sqrt{n}=\frac{z_{\alpha/2}\sqrt{2\pi}+z_\beta\sqrt{f-\delta^2}}{|\delta|}$. 2π is usually replaced by the discordant response rate f. That is, $\sqrt{n}=\frac{z_{\alpha/2}\sqrt{f}+z_\beta\sqrt{f-\delta^2}}{|\delta|}$.

Example: Consider the eye study described earlier. Let π_1 be the success rate on treatment 1 equal to 0.80. Let π_2 be the success rate on treatment 2 equal to 0.60. Let f be the discordant rate equal to 0.50 which is equal to $\pi_{1,0}+\pi_{0,1}$. For a 2-sided test, let $\alpha=0.05$, and the power be 0.90. Then, $\delta_1=\pi_1-\pi_2=0.20$, $\sqrt{n}=\frac{1.96\sqrt{0.50}+1.28\sqrt{0.50-(0.20)^2}}{0.20}=11.27\rightarrow n=128$.

12.7 Simple Linear Regression

Take the simple linear regression model with constant slope and intercept. The model statement is $y_i=\gamma+\theta_i+\epsilon_i, i=1,2,...,n$, where ϵ_i is iid $N(0,\sigma^2)$. The sums of squares are

$$s_{yy}=\sum_{i=1}^{n}(y_i-\bar{y})^2,\;\; s_{xx}=\sum_{i=1}^{n}(x_i-\bar{x})^2,\;\; s_{xy}=\sum_{i=1}^{n}(x_i-\bar{x})(y_i-\bar{y})=\sum_{i=1}^{n}(x_i-\bar{x})y_i.$$

The *slope estimator* is

$$\widehat{\theta}=\frac{s_{xy}}{s_{xx}}=\frac{\sum_{i=1}^{n}(x_i-\bar{x})y_i}{s_{xx}}.$$

The *mean and variance estimators* are

$$E(\widehat{\theta})=\theta,\;\; Var(\widehat{\theta})=\frac{\sigma_\epsilon^2}{s_{xx}}$$

The *standardized* of $\widehat{\theta}$ is

$$z=\frac{\widehat{\theta}-\theta}{\sigma_\epsilon/s_{xx}}.$$

The notation above is used in one of the sequential monitoring articles. Also note, $(x_i-\bar{x})(y_i-\bar{y})=(x_i-\bar{x})y_i-(x_i-\bar{x})\bar{y}$, $\sum_{i=1}^{n}(x_i-\bar{x})y_i-\bar{y}\sum_{i=1}^{n}x_i-\bar{x}=\sum_{i=1}^{n}(x_i-\bar{x})y_i-0$, $E(\widehat{\theta})=\sum_{i=1}^{n}\frac{(x_i-\bar{x})E(y_i)}{s_{xx}}$, $E(y_i)=\delta+\theta x_i$, $Var(y_i)=Var(\epsilon_i)=\sigma_\epsilon^2$.

$$\Rightarrow E(\widehat{\theta}) = \sum_{i=1}^{n} \frac{(x_i - \bar{x})(\delta + \theta x_i)}{s_{xx}} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})\delta + \sum_{i=1}^{n}(x_i - \bar{x})\theta x_i}{s_{xx}} =$$

$$\frac{\delta \sum_{i=1}^{n}(x_i - \bar{x}) + \theta \sum_{i=1}^{n}(x_i - \bar{x})x_i}{s_{xx}} = 0 + \frac{\theta \sum_{i=1}^{n}(x_i - \bar{x})(x_i - \bar{x})}{s_{xx}} = \theta \frac{s_{xx}}{s_{xx}} = \theta \Rightarrow \text{unbiased.}$$

Now find the variance of $\widehat{\theta}$.

$$\widehat{\theta} = \sum_{i=1}^{n} \left[\frac{(x_i - \bar{x})}{s_{xx}}\right] y_i,$$

$$Var(\widehat{\theta}) = \sum_{i=1}^{n} \left[\frac{(x_i - \bar{x})}{s_{xx}}\right]^2 Var(y_i) = \sum_{i=1}^{n} \frac{(x_i - \bar{x})^2}{s_{xx}^2}\sigma_\epsilon^2 = \sigma_\epsilon^2 \frac{\sum_{i=1}^{n}(x_i - \bar{x})^2}{s_{xx}^2} = \sigma_\epsilon^2 \frac{s_{xx}}{s_{xx}^2} = \sigma_\epsilon^2 \Rightarrow \text{ unbiased.}$$

12.7.1 Model for Clinical Trials

The model is $y_{ij} = \delta_i + \theta_i x_j + \epsilon_{ij}, j = 1, 2, .., k; i = 1, 2, ..., n$. k is the number of visits and n is the number of subjects. The model for subject 1 is $y_{1j} = \delta_1 + \theta_1 x_j + \epsilon_{1j}, j = 1, 2, .., k$. For the estimator of $\widehat{\theta}_1$ see page 25 of the handout. The model for subject 2 is $y_{2j} = \delta_2 + \theta_2 x_j + \epsilon_{2j}, j = 1, 2, .., k$. For the estimator of $\widehat{\theta}_2$ see page 25 of the handout.

$$Var(\widehat{\theta}_i) = Var\left[E(\widehat{\theta}_i|\theta_i) + E(Var(\widehat{\theta}_i|\theta_i)\right] = Var(\widehat{\theta}_i) + E\left[\frac{\sigma_\epsilon^2}{s_i}\right] = \sigma_\theta^2 + \frac{\sigma_\epsilon^2}{s_i}.$$

R (used in calculating the sample size) is $R = \frac{\sigma_\epsilon^2}{\sigma_\theta^2} = \frac{\text{within subject variabilities}}{\text{between subject variability}}$.

12.8 Comparing Slopes for 2 Treatment Groups

Group	Population Mean Slope	Sample Size
1	θ_1	n_1
2	θ_2	n_2

Reference page 29 of the text book. $E(\widehat{\delta}) = E[\widehat{\theta}_1 - \widehat{\theta}_2] = E(\widehat{\theta}_1) - E(\widehat{\theta}_2) = \theta_1 - \theta_2$, $Var(\widehat{\theta}_1 - \widehat{\theta}_2) = Var(\widehat{\theta}_1) + Var(\widehat{\theta}_2) = \frac{1}{\sum_{i=1}^{n_1} v_{1i}^{-1}} + \frac{1}{\sum_{i=1}^{n_2} v_{2i}^{-1}}$ $v_{i1}^{-1} = \sigma_\theta^2[1 + R/S_{1i}]$, $v_{i2}^{-1} = \sigma_\theta^2[1 + R/S_{2i}]$, Reference page 30 of the text book. Pages 28-30 are in error. On page 33 of the text book: $L_{1i} = k; L_{2i} = k$ (no missed visits). If $x_1 = 0$, then the calculation on page 33 of the text book is correct. On page 40, the response $(0, 0)$ and $(11, 1)$ do not say anything about the difference between treatment 1 and treatment 2. $H_0 : \Pi_1 = \Pi_2$. $\delta = \Pi_1 - \Pi_2 = (\Pi_{10} - \Pi_{11}) - (\Pi_{01} - \Pi_{11}) = \Pi_{10} - \Pi_{01}$ On page 42 of the text, $E(w) = \sum_{\forall w} wg(w) = \cdots$, $E(w^2) = \sum_{\forall w} w^2 g(w) = \cdots$, Another form of H_0 is $H_0 : \delta = 0$. The test statistic under H_0 is $z = \frac{\bar{w}-0}{\sqrt{\frac{f}{n}}}$ $z = \frac{\bar{w}-0}{\sqrt{\frac{2\bar{p}}{n}}}$ Continuing on to page 46 of the text book, $\mu_0 = E_{H_0}(\bar{w})$, $\mu_1 = E_{H_1}(\bar{w})$, $\delta = \mu_1 - \mu_0$, $\sigma_{0n}^2 = Var_{H_0}(\bar{w})$, $\sigma_{1n}^2 = Var_{H_1}(\bar{w})$, With $\mu_0 = 0$, and $\delta = 0$, $\mu_1 = \Pi_1 - \Pi_2$, $\delta = \Pi_1 - \Pi_2$, $\sigma_{0n}^2 = \frac{2\Pi}{n}$, $\sigma_{1n}^2 = \frac{f-\delta^2}{n}$.

12.9 Homework and Answers

1. Fizz Laboratories, a pharmaceutical company, has developed a new pain relief medication(drug #1) for patients suffering from arthritis. The new medication is to be compared with a commonly marketed medication (drug #2). Equal numbers of subjects will be allocated to the 2 groups. Each subject will be treated and asked one hour later to rate the medication as either "complete relief" or "less than complete relief." Based upon the literature, an investigator believes that the standard drug will produce about 40% positive responses (i.e. $p_2 = 0.40$). Answer the following in terms of a 5% level test of $H_0 : p_1 = p_2$, versus $H_1 : p_1 \neq p_2$.

a. What sample size ($n = n_1 + n_2$) is needed so the test has a power of 0.90 for detecting the difference $\delta_1 = 0.20$? ($\delta = p_1 - p_2$). **Answer:** $\delta_1 = p_1 - p_2 = p_1 - 0.40 = 0.20 \Rightarrow p_1 = 0.60$. $\bar{p} = \frac{p_1+p_2}{2} = \frac{0.60+0.40}{2} = 0.50$.

$$\sigma_{0n}^2 = Var_{H_0}(S_n) = \bar{p}(1-\bar{p})\left(\frac{1}{n_1} + \frac{1}{n_2}\right).$$

$$\sigma_{1n}^2 = Var_{H_1}(S_n) = \frac{p_1(1-p_1)}{n_1} + \frac{p_2(1-p_2)}{n_2} = \frac{0.60(0.40)}{n_1} + \frac{0.40(0.60)}{n_2}.$$

$\alpha = 0.05 \Rightarrow \frac{\alpha}{2} = 0.025$, and the power is $1-\beta \Rightarrow \beta = 0.10$. Using the equation: $|\delta_1| = z_{\alpha/2}\sigma_{0n} + z_\beta \sigma_{1n}$,

$$0.20 = z_{\alpha/2}\sqrt{(0.25)\left(\frac{1}{n_1} + \frac{1}{n_2}\right)} + z_\beta\sqrt{\frac{0.24}{n_1} + \frac{0.24}{n_2}}$$

$n_1 = n_2, \alpha_{0.025} = \pm 1.96, \alpha_{0.10} = 1.282$.

$$0.20 = 1.96\sqrt{(0.25)\left(\frac{1}{n_1} + \frac{1}{n_1}\right)} + 1.282\sqrt{\frac{0.24}{n_1} + \frac{0.24}{n_1}}$$

$0.20 = \frac{1.38593}{\sqrt{n_1}} + \frac{0.8882}{\sqrt{n_1}}$, $0.20\sqrt{n_1} = 1.38593 + 0.8882$, $0.20\sqrt{n_1} = 2.2741$, $\sqrt{n_1} = 11.3706$, $n_1 = 129.29 \Rightarrow n_2 = 129.29 \Rightarrow n = n_1 + n_2 = 260$.

b. If only $n = 200$ subjects can be recruited what will be the power of the test for detecting the difference $\delta_1 = 0.20$? **Answer:** $n = 200$

$$0.20 = 1.96\sqrt{(0.25)\left(\frac{1}{100} + \frac{1}{100}\right)} + z_\beta\sqrt{\frac{0.24}{100} + \frac{0.24}{100}}$$

$0.20 = 0.138593 + z_\beta(0.06928)$, $0.061407 = z_\beta(0.06928)$, $z_\beta = 0.8864$, The power is $1-\beta \approx 0.816$.

2. Consider a trial that involves repeated measures on $n = n_1 + n_2$ subjects over a follow-up period of length D with K equally spaced follow-up times, Assume:

   i. Each subject completes all follow-up visits.

   ii. Subjects are allocated equally to the two groups.

The difference $\widehat{\theta}_1 - \widehat{\theta}_2$ in slope estimators has variance

$$Var(\widehat{\theta}_1 - \widehat{\theta}_2) = \frac{4\sigma_\theta^2}{n}\left[1 + \frac{12R(k-1)}{D^2k(k+1)}\right]$$

The *amount of information* available for estimating $\theta_1 - \theta_2$ is

$$I = \frac{1}{Var(\widehat{\theta}_1 - \widehat{\theta}_2)} = \frac{n}{4\sigma_\theta^2\left[1 + \frac{12R(k-1)}{D^2k(k+1)}\right]}, k \geq 2.$$

The information varies with D, k, R and takes its maximum attainable value when k or D tend to ∞ (or $R = 0$). The maximum attainable value of I is $I_{\max} = n/4\sigma_\theta^2$. The ratio of I to $I_{\max}$ is

$$\frac{I}{I_{\max}} = \frac{1}{1 + \frac{12R(k-1)}{D^2k(k+1)}}$$

a. Construct a table showing how $(I/I_{\max}) \times 100$ varies as a function of k and R for a trial of duration $D = 3$ years. (Show the table for $k = 2, 4, 6, 8, 10$ and $R = 0.20, 1.0, 5.0$). **Answer:**

k	R	$I/I_{\max}$
2	0.2	95.74468
2	1	81.8181
2	5	47.36842
4	0.2	96.15385
4	1	83.333
4	5	50
6	0.2	96.92308
6	1	86.30137
6	5	55.75221
8	0.2	97.47292
8	1	88.52459
8	5	60.67416
10	0.2	97.86477
10	1	90.16393
10	5	64.70588

b. Using the table obtained in part (a), what general conclusion can be drawn concerning how the choice of k may depend on R. **Answer:** When k is constant and R increase, the ratio $I/I_{\max}$ decreases. As k increases and R is constant, $I/I_{\max}$ increases. In general choose k such that $R < k$ to maximize $I/I_{\max}$.

3. Let Y_1, Y_2 be *independent* binomial random variables with the following probability distributions: $f_i(y) = \binom{n_i}{y} p_i^y (1-p_i)^{n_i - y}, y = 0, 1, 2, ..., n_i; i = 1, 2$. Let $\widehat{p}_i = \frac{y_i}{n_i}$ denote the sample proportions for $i = 1, 2$. Assuming n_1 and n_2 are both large, $\widehat{p}_i$ has approximately a normal distribution with mean p_i and variance $\frac{p_i(1-p_i)}{n_i}$. If p_i is the probability that a subject in group i experiences a certain event during a particular time period, then $\theta = \frac{p_1}{p_2}$ is called the *relative risk* of experiencing that event.

   a. Let $\widehat{\theta} = \frac{\widehat{p}_1}{\widehat{p}_2}$ denote an estimator of θ. Use the δ method to determine the mean and variance of the limiting normal distribution of $\ln(\widehat{\theta})$, where $\ln(\cdot)$ denotes natural logarithm. (Note: $\ln(\widehat{\theta}) = \ln(\widehat{p}_1) - \ln(\widehat{p}_2)$).

   b. Use the result obtained in part (a) to give a general formula for $100(1-\alpha)\%$ confidence limits for $\ln(\theta)$. Then invert the limits to give a formula for confidence limits on θ.

4. Let S_n denote a general statistic that has approximately, if n is large, a normal distribution with mean $\mu = E(S_n)$ and variance $\sigma_n^2 = Var(S_n)$. Consider testing $H_0 : \mu = u_0$ versus the one-sided alternative $H_1 : \mu > \mu_0$. The test statistic is $z = \frac{S_N - \mu_0}{\sigma_{0n}}$ where $\mu_0 = E_{H_0}(S_n)$ and $\sigma_{0n}^2 = Var_{H_0}(S_n)$. If H_0 is true, then z has approximately a standard normal distribution. Thus, H_0 will be rejected at significance level α if $z_{\text{obs}} \geq z_\alpha$. Beginning with the definition of power, show that the sample size needed so the test has power $1 - -\beta$ for detecting the difference $\delta_1 = \mu_1 - \mu_0$ must satisfy the following equation: $|\delta_1| = z_\alpha \sigma_{0n} + z_\beta \sigma_{1n}$ where $\sigma_{1n}^2 = Var_{H_1}(S_n)$.

12.10 Dummy Variables

Corrections to the handout given. Listed are the dummy variables for Example 1:

$$V_{1,1,i} = \begin{cases} 1, & \text{if } (x_i, y_i) = (1,1) \\ 0, & \text{otherwise} \end{cases}$$

$$V_{1,2,i} = \begin{cases} 1, & \text{if } (x_i, y_i) = (1,0) \\ 0, & \text{otherwise} \end{cases}$$

$$V_{2,1,i} = \begin{cases} 1, & \text{if } (x_i, y_i) = (0,1) \\ 0, & \text{otherwise} \end{cases}$$

$$V_{2,2,i} = \begin{cases} 1, & \text{if } (x_i, y_i) = (0,0) \\ 0, & \text{otherwise} \end{cases}$$

$$n_{1,1} = \sum_{i=1}^{n} V_{1,1,i}, \;\; n_{1,2} = \sum_{i=1}^{n} V_{1,2,i}, \;\; n_{2,1} = \sum_{i=1}^{n} V_{2,1,i}, \;\; n_{2,2} = \sum_{i=1}^{n} V_{2,2,i}.$$

where i indexes the number of successes in n trials. Marginally (individually), it is clear $n_{1,1}$, $n_{1,2}$, $n_{2,1}$, $n_{2,2}$ have binomial distributions. $n_{1,1}$, $n_{1,2}$, $n_{2,1}$, and $n_{2,2}$ are independent.

12.11 2×2 Frequency Tables

2×2 frequency tables arise in a number of settings:

- Paired binary data (studied earlier).
- Analysis of survival rates.
- Comparing proportions across strata.

Our discussion concerns a parameter called *the odds ratio.* The logarithm of the odds ratio is closely related to the logistic transform, which has an important role in the analysis of binary data.

Outline:

1. Two distinct sampling models.
2. Different forms of the chi-square statistic.
3. Relationship to the standardized difference of two sample proportions.
4. The odds ratio: definition, interpretation, estimation, and confidence limits.
5. Fisher's exact test.
6. Comparing proportions across strata: the Mantel-Haenszel statistic.

2×2 frequency tables arise when sampling a single population or when independently sampling two populations.

Example: A sample of n individuals is selected from a certain population and, for each individual, a pair of response variables (x, y) is observed.

		Tumor Regression	
		Yes	No
Toxicity	Yes	a	b
	No	c	d

Example: In a sample of $n = n_1 + n_2$ subjects, suppose n_1 of them are randomly allocated to drug A and n_2 to drug B. A single response variable is observed for each subject.

		Nausea		
		Yes	No	
Drug	A	a	b	n_1
	B	c	d	n_2

The interpretation of the above two examples is different, but the statistics are calculated the same way.

Definition If the row *or* column totals are fixed through sampling, the *sampling model* is two independent binomial distributions. If neither the row nor the column totals are fixed through sampling, the *sampling model* is the multinomial distribution.

Notation:

		Column		
		1	2	
Row	1	n_{11}	n_{12}	$n_{1\cdot}$
	2	n_{21}	n_{22}	$n_{2\cdot}$

and the corresponding parameters

π_{11}	π_{12}	$\pi_{1\cdot}$
π_{21}	π_{22}	$\pi_{2\cdot}$
$\pi_{\cdot 1}$	$\pi_{\cdot 2}$	

With the multinomial sampling model, $\sum \pi_{i,j} = 1$ and $n_{11}+n_{12}+n_{21}+n_{22} = n$. With the binomial sampling model, $\pi_{11}+\pi_{12} = 1$, $\pi_{21}+\pi_{22} = 1$, and $n_{11}+n_{12} = n_{1\cdot}$, $n_{21}+n_{22} = n_{2\cdot}$ where $n_{1\cdot}$ and $n_{2\cdot}$ are sample sizes.

12.11.1 Binomial Sampling Model

n_{11} has a binomial distribution

$$f(n_{11}) = \left(\begin{array}{c} n_{1\cdot} \\ n_{11} \end{array} \right) (\pi_{11})^{n_{11}}(1-\pi_{11})^{n_{1\cdot}-n_{11}}, n_{11} = 0, 1, 2, ..., n_{1\cdot}.$$

n_{21} has a binomial distribution

$$g(n_{21}) = \left(\begin{array}{c} n_{2\cdot} \\ n_{21} \end{array} \right) (\pi_{21})^{n_{21}}(1-\pi_{21})^{n_{2\cdot}-n_{21}}, n_{21} = 0, 1, 2, ..., n_{2\cdot}.$$

where n_{11} and n_{21} are independent random variables.

12.11.2 Multinomial Sampling Model

For the multinomial model, the joint distribution is $f(n_{11}, n_{12}, n_{21}, n_{22}) = \frac{n!}{n_{11}!n_{12}!n_{21}!n_{22}!}(\pi_{11})^{n_{11}}(\pi_{12})^{n_{12}}(\pi_{21})^{n_{21}}(\pi_{22})^{n_{22}}$ where $n_{11}+n_{12}+n_{21}+n_{22} = n$, and $\sum \pi_{ij} = 1$.

12.11.3 Chi-Square Statistic

The standard chi-square statistic for testing homogeneity ($H_0 : \pi_{11} = \pi_{21}$) in two independent binomial populations or for testing independence ($H_0 : \pi_{11}\pi_{22} = \pi_{21}\pi_{12}$) in a multinomial population is $\chi^2 = \frac{(n_{11}n_{22}-n_{12}n_{21})^2 n}{n_{\cdot 1}n_{\cdot 2}n_{1\cdot}n_{2\cdot}}$ where if $n \to \infty$ or if $n_1, n_2 \to \infty$, then χ^2 has a limiting chi-square distribution with degrees of freedom of 1. Note that the numerator is a cross product difference and the denominator is the product of the marginal totals.

12.11.4 Continuity Correction

The continuity correction for the chi-square is $\chi^2 = \frac{(|n_{11}n_{22}-n_{12}n_{21}|-\frac{n}{2})^2 n}{n_{.1}n_{.2}n_{1.}n_{2.}}$.

12.11.5 Summary of the Chi-Square Statistics

The following summary applies to the chi-square statistics for 2×2 tables.

1. $\chi^2 = \frac{(n_{11}n_{22}-n_{12}n_{21})^2 n}{n_{.1}n_{.2}n_{1.}n_{2.}}$

2. The typical goodness-of-fit: $\chi^2 = \sum_{i,j} \frac{(n_{ij}-\hat{E}_{ij})^2}{\hat{E}_{ij}}$ where $\hat{E}_{11} = \frac{n_{.1}n_{1.}}{n}$, $\hat{E}_{12} = \frac{n_{.2}n_{1.}}{n}$, $\hat{E}_{21} = \frac{n_{.1}n_{2.}}{n}$, and $\hat{E}_{22} = \frac{n_{.2}n_{2.}}{n}$.

3. $\chi^2 = \frac{[n_{11}-E_{H_0}(n_{11})]^2}{Var_{H_0}(n_{11})}$ where $E_{H_0} = n_{1.}\frac{n_{.1}}{n}$, $Var_{H_0}(n_{11}) = \frac{n_{.1}n_{.2}n_{1.}n_{2.}}{n^2(n-1)}$.

4. $\chi^2 = \frac{[w(\hat{p}_1-\hat{p}_2)]^2}{\frac{nw\hat{p}(1-\hat{p})}{n-1}}$ where $w = \frac{n_{1.}n_{2.}}{n}$, $\hat{p}_1 = \frac{n_{11}}{n_{1.}}$, $\hat{p}_2 = \frac{n_{21}}{n_{2.}}$, $\hat{p} = \frac{n_{11}+n_{21}}{n}$,

Note that (1) and (2) are equivalent. (3) and (4) are equivalent, but slightly different from (1) and (2). (3) and (4) are closely related to the Mantel-Haenszel statistic that we will study later. It can be shown that, in (4), $\chi^2 = \frac{(n_{11}n_{22}-n_{12}n_{21})^2(n-1)}{n_{.1}n_{.2}n_{1.}n_{2.}}$. Thus, (3) and (4) differ from (1) and (2) only by n and $n-1$ in the numerator. If n is large, the all four equations are nearly identical. Later we will show that the difference between (1) or (2) and (3) or (4) is, for large samples, the difference between a conditional test and an unconditional test.

12.11.6 Relationship to the Standardized Differences

This section will cover the relationship of the chi-squares to the standardized differences of two sample proportions. In the binomial case, consider $H_0 : \pi_{11} = \pi_{21}$. Let $\hat{p}_1 = \frac{n_{11}}{n_{1.}}$, $\hat{p}_2 = \frac{n_{21}}{n_{2.}}$, and let $\hat{p} = \frac{n_{11}+n_{21}}{n}$, be the estimate of a common value of π_{11} and π_{21}. The standardized difference is

$$Z = \frac{\hat{p}_1 - \hat{p}_2}{\sqrt{\frac{\hat{p}(1-\hat{p})}{n_{1.}} + \frac{\hat{p}(1-\hat{p})}{n_{2.}}}}.$$

It has a approximate standard normal distribution under H_0. Thus,

$$Z^2 = \frac{(\hat{p}_1 - \hat{p}_2)^2}{\hat{p}(1-\hat{p})[\frac{1}{n_{1.}} + \frac{1}{n_{2.}}]}$$

has an approximate chi-square distribution with 1 degrees of freedom. It is easy to show that

$$Z^2 = \frac{n(n_{11}n_{22} - n_{12}n_{21})^2}{n_{1.}n_{2.}n_{.1}n_{.2}}$$

is the statistic found in (1) listed earlier.

12.11.7 The Odds Ratio

Let p denote the probability of getting a head when tossing a coin. The *odds* of getting a head, as opposed to not getting a head, is $\frac{p}{1-p}$. Thus, if $p = 0.40$, the odds of getting a head is $\frac{0.40}{0.60} = \frac{4}{6}$ or 4:6. Consider a 2×2 table with parameters

π_{11}	π_{12}
π_{21}	π_{22}

In row 1, the odds that the event in column 1 occurs is $\frac{\pi_{11}}{\pi_{12}} = \frac{\pi_{11}}{1-\pi_{11}}$. In row 2, the odds that the event in column 1 occurs is $\frac{\pi_{21}}{\pi_{22}} = \frac{\pi_{21}}{1-\pi_{21}}$.

Definition: The odds ratio, ψ is row 1 odds divided by row 2 odds. So, $\psi = \frac{\pi_{11}/\pi_{12}}{\pi_{21}/\pi_{22}} = \frac{\pi_{11}\pi_{22}}{\pi_{21}\pi_{12}}$

If the rows of the table represent independent binomial samples, then, $\pi_{11} + \pi_{12} = 1$ and $\pi_{21} + \pi_{22} = 1$ or $\pi_{12} = 1 - \pi_{11}$ and $\pi_{22} = 1 - \pi_{21}$. In this case, the odds ratio is $\psi = \frac{\pi_{11}\pi_{22}}{\pi_{21}\pi_{12}} = \frac{\frac{\pi_{11}}{1-\pi_{11}}}{\frac{\pi_{21}}{1-\pi_{21}}}$. If π_{11} and π_{21} are both small, the $\psi = \frac{\pi_{11}}{\pi_{21}}$ where the later quantity is called the *relative risk* of the event in column 1.

12.11.8 Odds Ratio Estimate

$\psi = \frac{\pi_{11}\pi_{22}}{\pi_{21}\pi_{12}}$. $\hat{\psi}$ is an estimate of ψ is $\hat{\psi} = \frac{\hat{\pi}_{11}\hat{\pi}_{22}}{\hat{\pi}_{21}\hat{\pi}_{12}}$. $\hat{\pi}_{ij} = \frac{n_{ij}}{n}$ is the sample proportion in row i and column j. Thus, $\hat{\psi} = \frac{n_{11}n_{22}}{n_{21}n_{12}}$.

Example: [Physician's Health Study (Meinert, 1986, page 314)] Take two independent binomials. The following table comes from a double blinded study with physicians as the participants.

	Myocardial Infarction		
	Attack	No Attack	
Placebo	189	10,845	11,034
Aspirin	104	10,933	11,037

The relative odds of a heart attack (placebo versus aspirin) is $\hat{\psi} = \frac{189(10{,}933)}{104(10{,}845)} = 1.83$. Thus, the odds of an attack in the placebo group is 1.83 times the odds in the aspirin group.

12.11.9 Properties of the Odds Ratio

Recall that ψ is the row 1 odds divided by the row 2 odds.

1. In general, $0 < \psi < \infty$.
2. When the row 1 odds is greater than the row 2 odds, $1 < \psi < \infty$.
3. When the row 1 odds is less than the row 2 odds, $0 < \psi < 1$.
4. ψ is estimated in the same way in the binomial and multinomial sampling models.
5. In the binomial model, ψ is a measure of *departure from homogeneous* rows. $\psi = \frac{\pi_{11}(1-\pi_{21})}{\pi_{21}(1-\pi_{11})}$.
   (a) $\psi = 1$ implies $\pi_{11} = \pi_{21}$.
   (b) $\psi < 1$ implies $\pi_{11} < \pi_{21}$.
   (c) $\psi > 1$ implies $\pi_{11} > \pi_{21}$.
6. In multinomial sampling, ψ is a *measure of association.*
   (a) $\psi = 1$ implies independent row and column categories.
   (b) $\psi < 1$ implies negative association.
   (c) $\psi > 1$ implies positive association.

   Those are measures of dependence and independence.

Proof of item (6): Let (x, y) have the following bivariate distribution.

		y		
		1	0	
x	1	π_{11}	π_{12}	$\pi_{1\cdot}$
	0	π_{21}	π_{22}	$\pi_{2\cdot}$
		$\pi_{\cdot 1}$	$\pi_{\cdot 2}$	

The marginal of x is

x	0	1
$f_1(x)$	$\pi_{2\cdot}$	$\pi_{1\cdot}$

The marginal of y is

y	0	1
$f_2(y)$	$\pi_{\cdot 2}$	$\pi_{\cdot 1}$

The expectations of x and y are as follow: $E(x) = \pi_{1\cdot} = \pi_{11} + \pi_{12}$, $E(y) = \pi_{\cdot 1} = \pi_{11} + \pi_{21}$, Thus the covariance is $Cov(x, y) = \pi_{11} - \pi_{1\cdot}\pi_{\cdot 1} = \pi_{11} - (\pi_{11} + \pi_{12})(\pi_{11} + \pi_{21}) = \pi_{11} - \pi_{11}^2 - \pi_{11}\pi_{12} - \pi_{12}\pi_{11} - \pi_{12}\pi_{21} = \pi_{11}(1 - \pi_{11} - \pi_{21} - \pi_{12}) - \pi_{12}\pi_{21} = \pi_{11}\pi_{22} - \pi_{12}\pi_{21} = \pi_{12}\pi_{21}\left[\frac{\pi_{11}\pi_{22}}{\pi_{12}\pi_{21}} - 1\right] = \pi_{12}\pi_{21}[\psi - 1]$. Assume that $0 < \pi_{ij} < 1$ for all (i, j). Then, $Cov(x, y) = 0 \Rightarrow \psi = 1$. $Cov(x, y) > 0 \Rightarrow \psi > 1$. $Cov(x, y) < 0 \Rightarrow \psi < 1$. All that remains to be shown is that $Cov(x, y) = 0 \Rightarrow x, y$ are independent. By a well known property of independence of random variables, we have, x, y are independent implies $Cov(x, y) = 0$. We need only show the converse. Note that $E(x) = P(x = 1) = \pi_{1\cdot}$ $E(y) = P(y = 1) = \pi_{\cdot 1}$ $E(xy) = P(x = 1 \text{ and } y = 1) = \pi_{11}$. Thus, $Cov(x, y) = E(xy) - E(x)E(y), \forall x, y \Rightarrow P(x = 1 \text{ and } y = 1) - P(x = 1)P(y = 1)$ and $Cov(x, y) = 0 \Rightarrow P(x = 1 \text{ and } y = 1) = P(x = 1)P(y = 1)$. We omit showing the other cases, although they follow by repeatedly using the law of complements.

12.11.10 Large Sample Confidence Limits

This section contains the derivation for confidence limits for 2×2 tables for the odds ratio. The following derivations only apply to a 2×2 table for either the multinomial or binomial sampling schemes. The maximum likelihood estimator of ψ is $\hat{\psi} = \frac{n_{11}n_{22}}{n_{21}n_{12}}$. The $\log\hat{\psi}$ has approximately a normal distribution with mean $\ln\psi$ and a standard deviation of $\hat{\sigma}_{\log\hat{\psi}} = \sqrt{\frac{1}{n_{11}} + \frac{1}{n_{12}} + \frac{1}{n_{21}} + \frac{1}{n_{22}}}$ as $n \to \infty$. Approximate $100(1-\alpha)\%$ confidence limits for $\ln\psi$ are $\ln\hat{\psi} \pm z_{\alpha/2}\hat{\sigma}_{\ln\hat{\psi}}$. or

$$P\left(-z_{\alpha/2} < \frac{\ln\hat{\psi} - \ln\psi}{\sqrt{\frac{1}{n_{11}} + \frac{1}{n_{12}} + \frac{1}{n_{21}} + \frac{1}{n_{22}}}} < z_{\alpha/2}\right)$$

Any n_{ij} that is small or close to zero should be replaced by $n_{ij} + 0.50$.

Example: [The Physician's Health Study] For very small p and large n, a Poisson distribution approximation will work, but a Normal distribution approximation will not work. From a previous section $\psi = 1.83$. $\log\hat{\psi} = 0.6043$ and $\hat{\sigma}_{\log\hat{\psi}} = \sqrt{\frac{1}{189} + \frac{1}{104} + \frac{1}{10{,}845} + \frac{1}{10{,}933}} = 0.12284$. The 95% confidence limits for $\ln\psi$ are $0.6043 \pm 1.96(0.12284)$ 0.6043 ± 0.2408 $0.3635 < \ln\psi < 0.8451$ or $1.44 \leq \psi \leq 2.33$. The odds of an heart attack in the placebo group relative to the aspirin group is estimated to lie between 1.44 and 2.33.

12.11.11 Basis for the Confidence Limit

The log odds ratio is a function of the sample proportions $\hat{\pi}_{11}, \hat{\pi}_{12}, \hat{\pi}_{21}$, and $\hat{\pi}_{22}$ which in turn are functions of the cell counts n_{11}, n_{12}, n_{21}, and n_{22}, which either have a multinomial distribution or arise from independent binomial distributions. Since $(\hat{\pi}_{11}, \hat{\pi}_{12}, \hat{\pi}_{21}, \hat{\pi}_{22})$ has a limiting multivariate normal distribution, the $\delta-$method can be used to determine the limiting normal distribution of $\log\hat{\psi} = \log\frac{\hat{\pi}_{11}\hat{\pi}_{22}}{\hat{\pi}_{21}\hat{\pi}_{12}}$.

12.12 Homework and Answers

1. Suppose each subject in a clinical trial can be classified by two factors, each of which is described by a vector (x, y) of random variables that has the following joint distribution.

y \ x	1	0
1	π_{11}	π_{12}
0	π_{21}	π_{22}

Now consider a sequence $(x_i, y_i), i = 1, 2, ..., n$ of iid random vectors corresponding to observing the response of n subjects. It will be convenient to introduce the following binary random variables.

$$V_{i11} = \begin{cases} 1, & \text{if } (x_i, y_i) = (1,1). \\ 0, & \text{otherwise.} \end{cases}, \quad V_{i12} = \begin{cases} 1, & \text{if } (x_i, y_i) = (1,0). \\ 0, & \text{otherwise.} \end{cases},$$

$$V_{i21} = \begin{cases} 1, & \text{if } (x_i, y_i) = (0,1). \\ 0, & \text{otherwise.} \end{cases}, \quad V_{i22} = \begin{cases} 1, & \text{if } (x_i, y_i) = (0,0). \\ 0, & \text{otherwise.} \end{cases}$$

Let $V_i' = (V_{i11}, V_{i12}, V_{i21}, V_{i22}), i = 1, 2, ..., n$ and note that $V_1, V_2, ..., V_n$ are iid random vectors.

(a) The covariance matrix of $V_i' = (V_{i11}, V_{i12}, V_{i21}, V_{i22})$ is

$$\Sigma = \begin{bmatrix} Var(V_{11}) & Cov(V_{11}, V_{12}) & Cov(V_{11}, V_{21}) & Cov(V_{11}, V_{22}) \\ Cov(V_{12}, V_{11}) & Var(V_{12}) & Cov(V_{12}, V_{21}) & Cov(V_{12}, V_{22}) \\ Cov(V_{21}, V_{11}) & Cov(V_{21}, V_{12}) & Var(V_{21}) & Cov(V_{21}, V_{22}) \\ Cov(V_{22}, V_{11}) & Cov(V_{22}, V_{12}) & Cov(V_{22}, V_{21}) & Var(V_{22}) \end{bmatrix}$$

where the entries have a certain order to facilitate solving Part (b) below. For example, $Cov(V_{11}, V_{12}) = E(V_{11}V_{12}) - E(V_{11})E(V_{12})$. But, $V_{11}V_{12} = 0$ because a single subject's response can not simultaneously fall into category $(1,1)$ and $(1,0)$. Thus, $Cov(V_{11}, V_{12}) = 0 - E(V_{11})E(V_{12}) = -E(V_{11})E(V_{12})$, $E(V_{11}) = P(V_{11} = 1) = \pi_{11}, E(V_{12}) = P(V_{12} = 1) = \pi_{12} \Rightarrow Cov(V_{11}, V_{12}) = -\pi_{11}\pi_{12}$. Complete the derivation of all entries of Σ. Solution: $E(V_{11}) = \pi_{11}, E(V_{12}) = \pi_{12}, E(V_{21}) = \pi_{21}, E(V_{22}) = \pi_{22}$, $E(V_{11}^2) = E(V_{11}) = \pi_{11}$, etc. $Var(V_{11}) = E(V_{11}^2) - [E(V_{11})]^2 = \pi_{11} - \pi_{11}^2 = \pi_{11}(1 - \pi_{11})$. Similarly, $Var(V_{12}) = \pi_{12}(1 - \pi_{12}), Var(V_{21}) = \pi_{21}(1 - \pi_{21})$, and $Var(V_{22}) = \pi_{22}(1 - \pi_{22})$. $Cov(V_{11}, V_{12}) = E(V_{11}V_{12}) - E(V_{11})E(V_{12}) = 0 - \pi_{11}\pi_{12} = -\pi_{11}\pi_{12}$, etc. Thus, the vector

$$\underline{V} = \begin{bmatrix} V_{11} \\ V_{12} \\ V_{21} \\ V_{22} \end{bmatrix}$$

has a covariance matrix

$$\Sigma = (\sigma_{ij}) = \begin{bmatrix} \pi_{11}(1 - \pi_{11}) & -\pi_{11}\pi_{12} & -\pi_{11}\pi_{21} & -\pi_{11}\pi_{22} \\ -\pi_{12}\pi_{11} & \pi_{12}(1 - \pi_{12}) & -\pi_{12}\pi_{21} & -\pi_{12}\pi_{22} \\ -\pi_{21}\pi_{11} & -\pi_{21}\pi_{12} & \pi_{21}(1 - \pi_{21}) & -\pi_{21}\pi_{22} \\ -\pi_{22}\pi_{11} & -\pi_{22}\pi_{12} & -\pi_{22}\pi_{21} & \pi_{22}(1 - \pi_{22}) \end{bmatrix}$$

(b) Let the vector of sample proportions $\widehat{\pi}_{ij} = n_{ij}/n$ be written in the form

$$\underline{\widehat{\pi}}_i = \begin{bmatrix} \widehat{\pi}_{11} \\ \widehat{\pi}_{12} \\ \widehat{\pi}_{21} \\ \widehat{\pi}_{22} \end{bmatrix}$$

which corresponds to the order used in deriving the covariance matrix in Part (a). Recall that the log of the odds ratio $\psi = \frac{\pi_{11}\pi_{22}}{\pi_{21}\pi_{12}}$ can be written as a function of $\pi_{11}, \pi_{12}, \pi_{21}, \pi_{22}$, say $\phi = \phi(\pi_{11}, \pi_{12}, \pi_{21}, \pi_{22})$ in the following way.
$\phi = \ln(\psi) = \ln(\pi_{11}) + \ln(\pi_{22}) - \ln(\pi_{12}) - \ln(\pi_{21})$. The δ method theorem states that $\widehat{\phi} = \ln(\widehat{\pi}_{11}) + \ln(\widehat{\pi}_{22}) - \ln(\widehat{\pi}_{12}) - \ln(\widehat{\pi}_{21})$. has approximately a normal distribution as $n \to \infty$ with mean of ϕ and variance $Var(\widehat{\phi}) = \frac{1}{n}\underline{a}'\Sigma\underline{a}$ where $a_1 = \frac{\partial\phi}{\partial\pi_{11}}$,$a_2 = \frac{\partial\phi}{\partial\pi_{12}}$, $a_3 = \frac{\partial\phi}{\partial\pi_{21}}$, $a_4 = \frac{\partial\phi}{\partial\pi_{22}}$, Simplify $\underline{a}'\Sigma\underline{a}$ to show that $Var(\widehat{\phi}) = \frac{1}{n}\left(\frac{1}{\pi_{11}} + \frac{1}{\pi_{12}} + \frac{1}{\pi_{21}} + \frac{1}{\pi_{22}}\right)$. Solution: $a_1 = \frac{\partial\phi}{\partial\pi_{11}} = \frac{1}{\pi_{11}}$, $a_2 = \frac{\partial\phi}{\partial\pi_{12}} = -\frac{1}{\pi_{12}}$, $a_3 = \frac{\partial\phi}{\partial\pi_{21}} = -\frac{1}{\pi_{21}}$, $a_4 = \frac{\partial\phi}{\partial\pi_{22}} = \frac{1}{\pi_{22}}$.

$$\underline{a}'\Sigma\underline{a} = [a_1, a_2, a_3, a_4]\begin{bmatrix} a_1\sigma_{11} + a_2\sigma_{12} + a_3\sigma_{13} + a_4\sigma_{14} \\ a_1\sigma_{21} + a_2\sigma_{22} + a_3\sigma_{23} + a_4\sigma_{24} \\ a_1\sigma_{31} + a_2\sigma_{32} + a_3\sigma_{33} + a_4\sigma_{34} \\ a_1\sigma_{41} + a_2\sigma_{42} + a_3\sigma_{43} + a_4\sigma_{44} \end{bmatrix} =$$

$$[a_1, a_2, a_3, a_4]\begin{bmatrix} (1-\pi_{11}) + \pi_{11} + \pi_{11} - \pi_{11} \\ -\pi_{12} - (1-\pi_{12}) + \pi_{12} - \pi_{12} \\ -\pi_{21} + \pi_{21} - (1-\pi_{21}) - \pi_{21} \\ -\pi_{22} + \pi_{22} + \pi_{22} + (1-\pi_{22}) \end{bmatrix} =$$

$$\left[\frac{1}{\pi_{11}}, -\frac{1}{\pi_{12}}, -\frac{1}{\pi_{21}}, \frac{1}{\pi_{22}}\right]\begin{bmatrix} 1 \\ -1 \\ -1 \\ 1 \end{bmatrix} = \sum\sum\frac{1}{\pi_{ij}}.$$

Thus, the asymptotic variance of $\log\widehat{\psi}$ is $\sigma^2 = \frac{1}{n}\sum\frac{1}{\pi_{ij}}$ which is estimated by
$\widehat{\sigma}^2 = \frac{1}{n}\sum\frac{1}{\widehat{\pi}_{ij}} = \frac{1}{n}\sum\frac{n}{n_{ij}} = \sum\frac{1}{n_{ij}}$.

2. The following data are from a study that compared two local anesthetics used in dental surgery to relive pain. The table below shows the numbers x_{ij} of subjects who reported no pain during surgery.

Kind of Surgery	Anesthetic # 1 n	x	Anesthetic # 2 n	x
1(Periodontic)	23	13	24	16
2(Endontic)	29	20	31	27

Assume that $\{x_{ij}\}$ are independent and have binomial distributions with sample sizes n_{ij} (indicated in the table) and with success probabilities θ_{ij}. That is, θ_{ij} is the probability that a subject in row i, column j suffers no pain. The two anesthetics represent different treatments while the kind of surgery is a factor with two levels. Recall that the logistic transform is
$\lambda_{ij} = \log\left(\frac{\theta_{ij}}{1-\theta_{ij}}\right)$.

(a) Let $\Delta_1 = \lambda_{11} - \lambda_{12}$ denote the log odds ratio for row 1 and let $\Delta_2 = \lambda_{21} - \lambda_{22}$ denote the log odds ratio for row 2. The model described above implies *that all observations in row 1 are independent of all observations in row 2.* Use this fact and our previous results on confidence limits for a single log odds ratio to give a general formula for confidence limits for $\Delta_1 - \Delta_2$. You will need to think of the data in rows 1 and 2 as consisting of two 2×2 tables.

	S	F
1	$n_{11}^{(1)}$	$n_{12}^{(1)}$
2	$n_{21}^{(1)}$	$n_{22}^{(1)}$
1	$n_{11}^{(2)}$	$n_{12}^{(2)}$
2	$n_{21}^{(2)}$	$n_{22}^{(2)}$

Solution:

$$\widehat{\Delta}_1 = \log\left(\frac{n_{11}^{(1)} n_{22}^{(1)}}{n_{21}^{(1)} n_{12}^{(1)}}\right)$$

Earlier we showed that $\widehat{\Delta}_1$ has a mean of

$$\Delta_1 = \log\left(\frac{\theta_{11}^{(1)}(1-\theta_{21}^{(1)})}{\theta_{21}^{(1)}(1-\theta_{11}^{(1)})}\right).$$

$$Var[\widehat{\Delta}_1] = \frac{1}{n_{11}^{(1)}} + \frac{1}{n_{12}^{(1)}} + \frac{1}{n_{21}^{(1)}} + \frac{1}{n_{22}^{(1)}}.$$

Similarly for the 2×2 table in row 2,

$$\widehat{\Delta}_2 = \log\left(\frac{n_{11}^{(2)} n_{22}^{(2)}}{n_{21}^{(2)} n_{12}^{(2)}}\right)$$

has a mean

$$\Delta_2 = \log\left(\frac{\theta_{11}^{(2)}(1-\theta_{21}^{(2)})}{\theta_{21}^{(2)}(1-\theta_{11}^{(2)})}\right).$$

$$Var[\widehat{\Delta}_2] = \frac{1}{n_{11}^{(2)}} + \frac{1}{n_{12}^{(2)}} + \frac{1}{n_{21}^{(2)}} + \frac{1}{n_{22}^{(2)}}.$$

Since $\widehat{\Delta}_1, \widehat{\Delta}_2$ are independent, $\widehat{\Delta}_1 - \widehat{\Delta}_2$ is asymptotically normal with a mean of $\Delta_1 - \Delta_2$ and a variance of

$$Var[\widehat{\Delta}_1 - \widehat{\Delta}_2] = \sum \frac{1}{n_{ij}^{(1)}} + \sum \frac{1}{n_{ij}^{(2)}}.$$

Thus, a general $100(1-\alpha)\%$ confidence interval for $\Delta_1 - \Delta_2$ is

$$\widehat{\Delta}_1 - \widehat{\Delta}_2 \pm \sqrt{\sum \frac{1}{n_{ij}^{(1)}} + \sum \frac{1}{n_{ij}^{(2)}}}.$$

(b) Use the given data to obtain a 95% confidence limit for $\Delta_1 - \Delta_2$. Solution: For the given data, we form the following 2×2 tables:

For Row 1:

	S	F	
1	13	10	23
2	16	8	24
	29	18	47

$\widehat{\Delta}_1 = \log\left(\frac{13(8)}{16(10)}\right) = -0.43$, $e_1 = E_{H_0}(n_{11}^{(1)}) = \frac{29(23)}{47} = 14.19$, $v_1 = Var_{H_0}(n_{11}^{(1)}) = \frac{29(18)(23)(24)}{(47)^2(46)} = 2.84$.

For Row 2:

	S	F	
1	20	9	29
2	27	4	31
	47	13	60

$\widehat{\Delta}_2 = \log\left(\frac{20(4)}{27(9)}\right) = -1.11$, $e_2 = E_{H_0}(n_{11}^{(2)}) = \frac{47(29)}{60} = 22.72$, $v_2 = Var_{H_0}(n_{11}^{(2)}) = \frac{47(13)(29)(31)}{(60)^2(59)} = 2.59$. Since the 95% confidence limits for $\Delta_1 - \Delta_2$ are $-0.43 - (-1.11) \pm 1.96$ $\sqrt{\left(\frac{1}{13} + \frac{1}{10} + \frac{1}{16} + \frac{1}{8}\right) + \left(\frac{1}{20} + \frac{1}{9} + \frac{1}{27} + \frac{1}{4}\right)} = 0.68 \pm 1.96\sqrt{0.813}$, $-1.09 < \Delta_1 - \Delta_2 < 2.45$.

(c) On the basis of the confidence limits in Part (b), is there any evidence of interaction between treatments and the kind of surgery? (Explain how you are using the confidence limits to arrive at a conclusion). Solution: Since zero is included between these limits, we have no evidence against the assumption $\Delta_1 - \Delta_2 = 0$. Conclusion: No evidence of interaction.

(d) Use the Mantel-Hanszel statistic to test, at significance level $\alpha = 0.05$ the hypothesis of no treatment difference (Show what you are doing). Solution: $H_0 : \Delta = 0$, versus $H_1 : \Delta \neq 0$, $\alpha = 0.05$ where Δ is the common log odds ratio of rows 1 and 2. The test statistic is $\chi^2 = \frac{(|S-E|-0.50)^2}{V}$ where $S = n_{11}^{(1)} + n_{11}^{(2)}$, $E = E_{H_0}(S)$, $V = Var_{H_0}(S)$. Reject H_0 if $\chi^2_{obs} \geq 3.84$. Conclusion: $S = 13 + 20 = 33$, $E = e_1 + e_2 = 14.19 + 22.72 = 36.91$, $V = v_1 + v_2 = 2.84 + 2.59 = 5.43$, $\chi^2_{obs} = \frac{(|33-36.91|-0.50)^2}{5.43} = 2.14$ Thus, do not reject the null hypothesis.

3. Let X, Y have independent binomial distributions,

$$P(X = x) = \binom{n_1}{x} (\theta_1)^x (1-\theta_1)^{n_1 - x}, x = 0, 1, ..., n_1,$$

$$P(Y = y) = \binom{n_2}{y} (\theta_2)^y (1-\theta_2)^{n_2 - y}, y = 0, 1, ..., n_2,$$

where $n_1 + n_2 = 7$. Consider the problem of testing $H_0 : \theta_1 = \theta_2$ versus $H_1 : \theta_1 < \theta_2$ at the significance level $\alpha = 0.02$. When using the Fisher exact test, the rejection region is left tailed and consists of rejecting H_0 whenever the conditional p-value is less-than or equal to 0.02 where the p-value is equal to $P_{H_0}(X \leq x_{obs}|S = s)$, where x_{obs} is the observed value of x and s is the observed value of $S = x+y$.

(a) Use the attached table to determine the p-value when $x_{obs} = 0$ and $s = 6$. Solution: $p - value = P_{H_0}(X \leq 0|s = 6) = \frac{7}{3003}$.

(b) Note that $x = 0$ and $s = 6$ corresponds to the (x, y) pair $x = 0$, and $y = 6$ (because $y = s - x$). Use the attached table to determine the set, denoted by $W_{0.02}$, of all (x, y) pairs for which H_0 will be rejected at $\alpha = 0.02$ (i.e. all (x, y) pairs for which the p-value is less than or equal to 0.02). The set $W_{0.02}$ contains 6 pairs. Solution: $W_{0.02} = \{(0, 5), (0, 6), (0, 7), (1, 6), (1, 7), (2, 7)\}$ These outcomes occur when $s = 5, 6, 7, 8, 9$ and result in rejecting H_0 at the level $\alpha = 0.02$.

(c) The set $W_{0.02}$ is the rejection region of an $\alpha = 0.02$ level test. Thus the power of the test is the probability, calculated under the assumption of specific values of $\theta_1 < \theta_2$, that (x, y) takes a value in the set $W_{0.02}$. Determine the power of the test at the specific alternative $\theta_1 = 0.20$ and $\theta_2 = 0.80$. Hint: The power is $\sum_{(x,y)\in W_{0.02}} P(X = x, Y = y)$. The terms of this sum are easy to calculate. $\phi(0.20, 0.80) = P_{0.20}(X = 0)P_{0.80}(Y = 5) + P_{0.20}(X = 0)P_{0.80}(Y = 6)+ P_{0.20}(X = 0)P_{0.80}(Y = 7) + P_{0.20}(X = 1)P_{0.80}(Y = 6)+ P_{0.20}(X = 1)P_{0.80}(Y = 7) + P_{0.20}(X = 2)P_{0.80}(Y = 7)$.

$$P_{0.20}(X = 0) = \begin{pmatrix} 7 \\ 0 \end{pmatrix} (0.20)^0(0.80)^7 = 0.2097,$$

$$P_{0.20}(X = 1) = \begin{pmatrix} 7 \\ 1 \end{pmatrix} (0.20)^1(0.80)^6 = 0.3670,$$

$$P_{0.20}(X = 2) = \begin{pmatrix} 7 \\ 2 \end{pmatrix} (0.20)^2(0.80)^5 = 0.2753,$$

$$P_{0.80}(X = 5) = \begin{pmatrix} 7 \\ 5 \end{pmatrix} (0.80)^5(0.20)^2 = 0.2753,$$

$$P_{0.80}(X = 6) = \begin{pmatrix} 7 \\ 6 \end{pmatrix} (0.80)^6(0.20)^1 = 0.3670,$$

$$P_{0.80}(X = 7) = \begin{pmatrix} 7 \\ 7 \end{pmatrix} (0.80)^7(0.20)^0 = 0.2097.$$

Then, $\phi(0.20, 0.80) = 0.2097(0.2753) + (0.2097)(0.3670)+ (0.2097)(0.2097) + 0.3670(0.3670) + 0.3670(0.2097)+ (0.2753)(0.2097) = 0.4480$.

4. The formula given in class for large sample confidence limits for the log odds ratio, $\log \psi$ is

$$\log \widehat{\psi} \pm z_{\alpha/2}\sqrt{\frac{1}{n_{11}} + \frac{1}{n_{21}} + \frac{1}{n_{12}} + \frac{1}{n_{22}}}.$$

This formula, however, was derived under the assumption that $n_{11}, n_{21}, n_{12}, n_{22}$ has a multinomial distribution and $n \to \infty$. Assume that n_{11} and n_{21} have independent binomial distributions: $f_1(n_{11}) = \begin{pmatrix} n_{1\cdot} \\ n_{11} \end{pmatrix} (\pi_{11})^{n_{11}}(1-\pi_{11})^{n_{1\cdot}-n_{11}}, n_{11} = 0, 1, 2, ..., n_{1\cdot}$. $f_2(n_{21}) = \begin{pmatrix} n_{2\cdot} \\ n_{21} \end{pmatrix} (\pi_{21})^{n_{21}}(1-\pi_{21})^{n_{2\cdot}-n_{21}}, n_{21} = 0, 1, 2, ..., n_{2\cdot}$. The log odds ratio
$\phi = \ln(\psi) = \ln\left[\frac{\pi_{11}}{1-\pi_{11}}\right] - \ln\left[\frac{\pi_{21}}{1-\pi_{21}}\right]$ is estimated by $\widehat{\phi} = \ln(\widehat{\psi}) = \ln\left[\frac{\widehat{\pi}_{11}}{1-\widehat{\pi}_{11}}\right] - \ln\left[\frac{\widehat{\pi}_{21}}{1-\widehat{\pi}_{21}}\right]$ which is the difference of two independent random variables.

(a) Use the δ method to get the mean and variance of the approximate normal distribution of $\widehat{\phi}$. Solution: Let $\phi(x) = \ln\left(\frac{x}{1-x}\right)$. Then, $\phi'(x) = \frac{1}{x(1-x)}$.

$$Var[\phi(\widehat{\pi}_{11})] = [\phi'(\widehat{\pi}_{11})]^2 \frac{\pi_{11}(1-\pi_{11})}{n_{1\cdot}} = \left[\frac{1}{\pi_{11}(1-\pi_{11})}\right]^2 \frac{\pi_{11}(1-\pi_{11})}{n_{1\cdot}} = \frac{1}{n_{1\cdot}\pi_{11}(1-\pi_{11})}.$$

$$Var[\phi(\widehat{\pi}_{21})] = [\phi'(\widehat{\pi}_{21})]^2 \frac{\pi_{21}(1-\pi_{21})}{n_{2\cdot}} = \left[\frac{1}{\pi_{21}(1-\pi_{21})}\right]^2 \frac{\pi_{21}(1-\pi_{21})}{n_{2\cdot}} = \frac{1}{n_{2\cdot}\pi_{21}(1-\pi_{21})}.$$

Thus,

$$\ln(\widehat{\psi}) = \ln\left[\frac{\widehat{\pi}_{11}}{1-\widehat{\pi}_{11}}\right] - \ln\left[\frac{\widehat{\pi}_{21}}{1-\widehat{\pi}_{21}}\right]$$

is the difference of independent random variables and has a variance

$$\sigma^2 = Var[\ln\widehat{\psi}] = \frac{1}{n_{1\cdot}\pi_{11}(1-\pi_{11})} + \frac{1}{n_{2\cdot}\pi_{21}(1-\pi_{21})}$$

which is estimated by

$$\widehat{\sigma}^2 = \frac{1}{n_{1\cdot}\left(\frac{n_{11}}{n_{1\cdot}}\right)\left(\frac{n_{12}}{n_{1\cdot}}\right)} + \frac{1}{n_{2\cdot}\left(\frac{n_{21}}{n_{2\cdot}}\right)\left(\frac{n_{22}}{n_{2\cdot}}\right)} = \frac{n_{1\cdot}}{n_{11}n_{12}} + \frac{n_{2\cdot}}{n_{21}n_{22}} = \frac{(n_{11}+n_{12})}{n_{11}n_{12}} + \frac{(n_{21}+n_{22})}{n_{21}n_{22}} =$$

$$\frac{1}{n_{11}} + \frac{1}{n_{21}} + \frac{1}{n_{12}} + \frac{1}{n_{22}}$$

(b) Show that $\log\widehat{\psi}$ still applies in the case of independent binomial samples. Solution: The $100(1-\alpha)\%$ confidence limits for $\log\psi$ are

$$\log\widehat{\psi} \pm z_{\alpha/2}\sqrt{\frac{1}{n_{11}} + \frac{1}{n_{21}} + \frac{1}{n_{12}} + \frac{1}{n_{22}}}$$

which is the same as before.

12.13 Comparing Two Population Proportions

From now on, we assume binomial sampling in which subjects are randomly allocated to two treatment groups.

		Response		
		S	F	
Trt	1	x	$n_1 - x$	n_1
	2	y	$n_2 - y$	n_2

where x is the number of successes among the n_1 subjects allocated to treatment 1, and y is the number of successes among the n_2 subjects allocated to treatment 2. x and y have independent binomial distributions. The marginal distributions are

$$f_1(x) = \binom{n_1}{x}\theta_1^x(1-\theta_1)^{n_1-x}, x = 0, 1, 2, ..., n_1.$$

$$f_2(y) = \begin{pmatrix} n_2 \\ y \end{pmatrix} \theta_2^y (1-\theta_2)^{n_2-y}, y = 0, 1, 2, ..., n_2.$$

12.13.1 Odds Ratio

The odds ratio is $\psi = \frac{\frac{\theta_1}{1-\theta_1}}{\frac{\theta_2}{1-\theta_2}}$ where the numerator is the odds of success in row 1 and the denominator is the odds of success in row 2.

12.13.2 Log Odds Ratio

The log odds ratio is given by $\Delta = \log\psi = \log\frac{\theta_1}{1-\theta_1} - \log\frac{\theta_2}{1-\theta_2}$ where Δ can be interpreted as a parameter indicating a treatment effect in the sense that $\Delta = 0 \Rightarrow \theta_1 = \theta_2 \Rightarrow$ No treatment effect. $\Delta > 0 \Rightarrow \theta_1 > \theta_2 \Rightarrow$ Treatment 1 produces a higher success rate than 2. $\Delta < 0 \Rightarrow \theta_1 < \theta_2 \Rightarrow$ Treatment 2 produces a higher success rate than 1.

12.13.3 The Likelihood Function

The likelihood function is

$$h(x,y) = \begin{pmatrix} n_1 \\ x \end{pmatrix} \theta_1^x (1-\theta_1)^{n_1-x} \begin{pmatrix} n_2 \\ y \end{pmatrix} \theta_2^y (1-\theta_2)^{n_2-y} =$$

$$\begin{pmatrix} n_1 \\ x \end{pmatrix} \begin{pmatrix} n_2 \\ y \end{pmatrix} (\frac{\theta_1}{1-\theta_1})^x (\frac{\theta_2}{1-\theta_2})^y (1-\theta_1)^{n_1} (1-\theta_2)^{n_2}.$$

12.13.4 Re parameterization

Re parameterizing the likelihood function can be done as follow. Let $\Delta = \lambda_1 - \lambda_2$ where, by the logistic transform,

$$\lambda_1 = \log\frac{\theta_1}{1-\theta_1} \Rightarrow \frac{\theta_1}{1-\theta_1} = e^{\lambda_1} \text{ and } 1-\theta_1 = \frac{1}{1+e^{\lambda_1}},$$

$$\lambda_2 = \log\frac{\theta_2}{1-\theta_2} \Rightarrow \frac{\theta_2}{1-\theta_2} = e^{\lambda_2} \text{ and } 1-\theta_2 = \frac{1}{1+e^{\lambda_2}}$$

12.13.5 Re parameterizing the Likelihood Function

The joint likelihood function of x, y is

$$h(x,y) = f_1(x) f_2(y) = \frac{\begin{pmatrix} n_1 \\ x \end{pmatrix} \begin{pmatrix} n_2 \\ y \end{pmatrix} e^{x\lambda_1 + y\lambda_2}}{(1+e^{\lambda_1})^{n_1}(1+e^{\lambda_2})^{n_2}}.$$

Let $\phi = \lambda_2$ and $\Delta = \lambda_1 - \lambda_2$. Substituting $\lambda_2 = \phi$ and $\lambda_1 = \phi + \Delta$ gives

$$h(x,y) = \frac{\begin{pmatrix} n_1 \\ x \end{pmatrix} \begin{pmatrix} n_2 \\ y \end{pmatrix} e^{x\Delta + (x+y)\phi}}{(1+e^{\phi+\Delta})^{n_1}(1+e^{\phi})^{n_2}}.$$

The parameter space $\{(\theta_1, \theta_2) : 0 < \theta_i < 1, i = 1, 2\}$ is mapped one-to-one to the new parameter space $\{(\phi, \Delta) : -\infty < \phi < \infty, -\infty < \Delta < \infty\}$ where Δ is the treatment effect on a logistic scale, and ϕ is a nuisance parameter.

12.13.6 Fisher's Exact Test

Fisher's test is based on the conditional distribution of x given $S = s$ where $S = x+y$. The joint distribution of (x, y) is

$$h(x,y) = \frac{\binom{n_1}{x}\binom{n_2}{y} e^{x\Delta+(x+y)\phi}}{(1+e^{\phi+\Delta})^{n_1}(1+e^{\phi})^{n_2}}.$$

The marginal distribution of S is

$$g(s) = P(S = s) = \sum_{\{(x,y):x+y=s\}} h(x,y) = \sum_{x=a}^{b} \frac{\binom{n_1}{x}\binom{n_2}{s-x} e^{x\Delta+\phi s}}{(1+e^{\phi+\Delta})^{n_1}(1+e^{\phi})^{n_2}}$$

when s is fixed at its observed value. The range of x is $a \le x \le b$ where $a = \max(0, s-n_2)$, and $b = \min(n_1, s)$. To see this, note that $x \le s$ and $x \le n_1$ implies that $x \le \min(s, n_1) = b$. Also, $s - x = y$. So, $y = s - x \le n_2$ implies that $x \ge s - n_2$ and $x \ge 0$ which implies that $x \ge \max(0, s - n_2) = a$. We have $a \le x \le b$ where $a = \max(0, s - n_2)$ and $b = \min(s, n_1)$.

12.13.7 Conditional Distribution of $x|S = s$

$$h(x|s) = \frac{h(x, s-x)}{g(s)}, a \le x \le b,$$

$$\frac{\binom{n_1}{x}\binom{n_2}{s-x} e^{x\Delta}}{\sum_{u=a}^{b}\binom{n_1}{u}\binom{n_2}{s-u} e^{u\Delta}}, a \le x \le b$$

Note that $h(x|s)$ does not depend on ϕ. This distribution is called a *generalized hyper geometric* distribution. When $\Delta = 0$, the denominator is

$$\sum_{u=a}^{b}\binom{n_1}{u}\binom{n_2}{s-u} = \binom{n_1+n_2}{s}, a \le x \le b,$$

which follows from a combinatorial identity.

12.13.8 The Null Distribution

Under $H_0 : \Delta = 0$, the distribution of x given $S = s$ is

$$h_0(x|s) = \frac{\binom{n_1}{x}\binom{n_2}{s-x}}{\binom{n_1+n_2}{s}}, a \le x \le b,$$

which is the ordinary hyper geometric distribution. That is, under H_0, x is distributed like the total number of successes occurring in a sample of size s taken *without replacement* from a population containing n_1 objects labeled S and n_2 objects labeled F.

12.13.9 Null Mean and Variance

$$E_{H_0}(x|s) = s\frac{n_1}{n},$$
$$Var_{H_0}(x|s) = \frac{n-s}{n-1}(s)\left(\frac{n_1}{n}\right)\left(\frac{n_2}{n}\right)$$

where $\frac{n-s}{n-1}$ is called the finite population correction factor. Note the similarity and differences between this mean and variance in comparison to the mean and variance of a binomial random variable.

12.13.10 Relationship to a 2×2 Table

Since we will often need to calculate the null mean and variance in the context of a 2×2 table, we now note the following relationship: $E_{H_0}(x|s) = s\frac{n_{.1}}{n}$, and $Var_{H_0}(x|s) = \frac{n-s}{n-1}(s)\left(\frac{n_{.1}}{n}\right)\left(\frac{n_{.2}}{n}\right)$. Then, $Var_{H_0}(x|s) = \frac{(n-s)(s)n_{.1}n_{.2}}{n^2(n-1)}$ which is the product of the marginal totals divided by $n^2(n-1)$.

12.13.11 The Likelihood Ratio Test

$H_0 : \Delta = 0$, versus $H_A : \Delta = \Delta_1$. The test statistic is

$$\frac{h(x|s,\Delta_1)}{h_0(x|s)} = \frac{\dfrac{\binom{n_1}{x}\binom{n_2}{s-x}e^{x\Delta_1}}{\sum_{u=a}^{b}\binom{n_1}{u}\binom{n_2}{s-u}e^{u\Delta_1}}}{\dfrac{\binom{n_1}{x}\binom{n_2}{s-x}}{\binom{n_1+n_2}{s}}} = c_s(\Delta_1)e^{x\Delta_1}.$$

The ratio increases in x if $\Delta_1 > 0 \Rightarrow$ reject H_0 if $x \geq c_1$. The ratio decreases in x if $\Delta_1 < 0 \Rightarrow$ reject H_0 if $x \leq c_2$. Thus, the alternative hypotheses are $H_A : \Delta > 0 \Rightarrow$ reject H_0 if $x \geq c_1$. $H_A : \Delta < 0 \Rightarrow$ reject H_0 if $x \leq c_2$. $H_A : \Delta \neq 0 \Rightarrow$ reject H_0 if $x \geq c_1$ or if $x \leq c_2$.

12.13.12 Large Sample Conditional Tests

As n increases and s also increases,

$$Z = \frac{X - E_{H_0}(x|s)}{\sqrt{Var_{H_0}(x|s)}}$$

converges to a standard normal distribution.

Example:

		Tumor Regression		
		Yes	No	
Trt	1	14	36	50
	2	8	42	50

Here, $s = 14 + 8 = 22$ where $x = 14$ is the number of successes observed for Fisher's test. Let θ_i be the population proportion of subjects that experience tumor regression under treatment $i, i = 1, 2$. The hypotheses are $H_0 : \theta_1 = \theta_2$ versus $H_A : \theta_1 > \theta_2$. These hypotheses are the same as $H_0 : \Delta = 0$ versus $H_0 : \Delta > 0$ where

$$\Delta = \log\left[\frac{\theta_1(1-\theta_1)}{\theta_2(1-\theta_2)}\right]$$

1. Use the standard test for comparing two population proportions. Solution: The test statistic is

$$Z = \frac{\hat{\theta}_1 - \hat{\theta}_2}{\hat{\theta}(1-\hat{\theta})\left(\frac{1}{n_1}+\frac{1}{n_2}\right)}.$$

Reject H_0 if $Z_{obs} \geq 1.65 = z_\alpha$. So, $\hat{\theta}_1 = \frac{14}{50} = 0.28$, $\hat{\theta}_2 = \frac{8}{50} = 0.16$, $\hat{\theta} = \frac{14+8}{50+50} = 0.22$, $Z_{obs} = \frac{0.28-0.16}{\sqrt{0.22(0.78)\left(\frac{1}{50}+\frac{1}{50}\right)}} = 1.45$, thus, do not reject H_0.

2. Use Fisher's exact test and the normal approximation for comparing two population proportions. Solution: The test statistic is $Z = \frac{X - E_{H_0}(x|s)}{\sqrt{Var_{H_0}(x|s)}}$. Reject H_0 if $Z_{obs} \geq 1.65 = Z_\alpha$. Conclusion, $x = 14$,

$$E_{H_0}(x|s) = s\left(\frac{n_1}{n}\right) = 22\left(\frac{50}{100}\right) = 11,$$

$$Var_{H_0}(x|s) = \frac{n-s}{n-1}(s)\left(\frac{n_1}{n}\right)\left(\frac{n_2}{n}\right) = \frac{100-22}{99}(22)\left(\frac{50}{100}\right)\left(\frac{50}{100}\right) \Rightarrow \sqrt{Var_{H_0}(x|s)} = 2.08.$$

$Z_{obs} = \frac{14-11}{2.08} = 1.44$; Thus, do not reject H_0.

It would be surprising if these tests did not agree; squaring each test statistic yields one of the chi-square statistics mentioned earlier.

12.13.13 Small Sample Case of Fisher's Exact Test

Small sample yield tests have low power; and therefore, we only briefly discuss this case.

		Tumor Regression		
		Yes	No	
Trt	1	1	4	5
	2	4	1	5

$H_0: \theta_1 = \theta_2$ versus $H_A: \theta_1 < \theta_2$. Reject H_0 if $x_{obs} \leq c$. $x_{obs} = 1$. The p-value is given by

$$P_{H_0}(x \leq 1|s=5) = h_0(x|s=5) = \frac{\binom{n_1}{x}\binom{n_2}{s-x}}{\binom{n_1+n_2}{s}} = \frac{\binom{5}{x}\binom{5}{s-x}}{\binom{10}{5}}, x = 0,1,2,...,5.$$

The the p-value is

$$\sum_{x=0}^{1} h_0(x|s=5) = \frac{\binom{5}{0}\binom{5}{5}}{\binom{10}{5}} + \frac{\binom{5}{1}\binom{5}{4}}{\binom{10}{5}} = \frac{26}{252} = 0.103.$$

Since the p-value is greater than 0.05, do not reject H_0. At *the nominal significance level* of 0.05, a test of $H_0: \psi = 1$ versus $H_A: \psi < 1$ rejects H_0 only for the (x, y) pairs $w_{0.05} = \{(0,4),(0,5),(1,5)\}$.

12.14 Example of Grouping by an Explanatory Variable

Question: Since the choice of strata (i.e. blocks) is somewhat arbitrary and can be selected in such a way as to affect the conclusion concerning a treatment difference, isn't it always best to use pre-stratification? Answer:

1. Peto, et. al. (1976, 1977) recommend post-stratification in large trials.
2. Our text book (page 69) points out that post-stratification is nearly as efficient (i.e. little loss in power) as pre-stratification.
3. It is often possible to select specific covariates out of a larger set to achieve a desired result (text book, bottom of page 301). For this reason, the process of selecting covariates to be used in an adjustment should be specified in the study protocol and adhered to in the primary analysis (text book, page 302).

Consider the following calculations.

Clinic	Group 1	Group 2	Log Odds Ratio
1	$x_{11} = 4M$	$x_{12} = 8M$	$\widehat{\Delta}_1 = \widehat{\lambda}_{11} - \widehat{\lambda}_{12} = -0.188$
	$n_{11} = 7M$	$n_{12} = 13M$	
	$\widehat{\theta}_{11} = \frac{4M}{7M} = 0.57$	$\widehat{\theta}_{12} = \frac{8M}{13M} = 0.62$	
	$\widehat{\lambda}_{11} = 0.282$	$\widehat{\lambda}_{12} = 0.470$	
2	$x_{21} = 2M$	$x_{22} = 12M$	$\widehat{\Delta}_2 = \widehat{\lambda}_{21} - \widehat{\lambda}_{22} = -0.164$
	$n_{21} = 5M$	$n_{22} = 27M$	
	$\widehat{\theta}_{21} = \frac{2M}{5M} = 0.40$	$\widehat{\theta}_{22} = \frac{12M}{27M} = 0.44$	
	$\widehat{\lambda}_{21} = -0.405$	$\widehat{\lambda}_{22} = -0.241$	

where the log odds ratio is given by $\widehat{\lambda}_{ij} = \log\left[\frac{\widehat{\theta}_{ij}}{1-\widehat{\theta}_{ij}}\right]$. Notes: 1) $\widehat{\theta}_{11} < \widehat{\theta}_{12}$ implies a treatment effect exists. $\widehat{\theta}_{21} < \widehat{\theta}_{22}$ implies that within clinic effect exists. 2) $\widehat{\theta}_1 = \frac{4M+2M}{7M+5M} = 0.50$ and $\widehat{\theta} = \frac{8M+12M}{13M+27M} = 0.50$ implies that if we do not stratify by clinics, we will not be able to detect a treatment difference.

Summary of the Logistic Model for Comparing Proportions in a 2 Factor Experiment

Consider the optimal allocation problem in Kokan (1963) for two samples (called strata) with two variables of interest. The problem can be solved using Lagrange multipliers. We wish to maximize $\phi = -(n_1 + n_2)$ subject to two linear inequalities f_1 and f_2. Using the Lagrange multiplier for $\phi + \lambda f_1$ yields the solution for the two equations for n_1 and n_2.

The layout of the data is given in the following table.

Row	Trt 1	Trt 2	
1	x_{11}	x_{12}	$\Delta_1 = \lambda_{11} - \lambda_{12}$
	n_{11}	n_{12}	
	θ_{11}	θ_{12}	
2	x_{21}	x_{22}	$\Delta_2 = \lambda_{21} - \lambda_{22}$
	n_{21}	n_{22}	
	θ_{21}	θ_{22}	
$\vdots k$	x_{k1}	x_{k2}	$\Delta_k = \lambda_{k1} - \lambda_{k2}$
	n_{k1}	n_{k2}	
	θ_{k1}	θ_{k2}	

The general model is x_{ij} independent, binomials, with sample sizes of n_{ij}, and with parameters θ_{ij}. The logistic transform is $\lambda_{ij} = \log\left[\frac{\theta_{ij}}{1-\theta_{ij}}\right]$. The treatment effects are measured by $\Delta_i = \lambda_{i1} - \lambda_{i2}$ which is the log odds ratio for row i. The full model is given by $\lambda_{i2} = \alpha_i$ where α_i is the row effects, and $\lambda_{i1} = \alpha_i + \Delta_i$ where Δ_i is the treatment effects. The model with no row by treatment interaction is $\lambda_{1i} = \alpha_i + \Delta$, and $\lambda_{2i} = \alpha_i$. The row effects α_i are nuisance parameters; the main parameter of interest is Δ. The likelihood function is

$$L(\alpha_1, \alpha_2, ..., \alpha_k, \Delta) = \prod_{i=1}^{k} \frac{\binom{n_{i1}}{x_{i1}}\binom{n_{i2}}{x_{i2}} e^{x_{i1}\Delta + \alpha_i s_i}}{(1+e^{\alpha_i+\Delta})^{n_{i1}}(1+e^{\alpha_i})^{n_{i2}}}$$

The sufficient statistic for the likelihood function L is $(W, s_1, s_2, ..., s_k)$ where $W = \sum_{i=1}^{k} x_{i1}, s_1 = x_{11} + x_{12}, s_2 = x_{21} + x_{22}, ..., s_k = x_{k1} + x_{k2}$. The s's are the total number of successes.

The Distribution of W Conditional on $S_1 = s_1, S_2 = s_2, ..., S_k = s_k$

W is distributed conditionally as a sum of independent random variables $x_{i1}, i = 1, 2, ..., k$ each having the following distributions.

$$f_i(x|\Delta, s_i) = P(x_{i1} = x|S_i = s_i) = \frac{\binom{n_{i1}}{x}\binom{n_{i2}}{s_i - x} e^{\Delta x}}{\sum_{u=a_i}^{b_i}\binom{n_{i1}}{u}\binom{n_{i2}}{s_i - u} e^{\Delta x u}}, a_i \leq x \leq b_i,$$

where $a_i = \max(0, s_i - n_{i2})$ and $b_i = \min(s_i, n_{i1})$ We know this from our previous study of Fisher's exact test.

Null Distribution of W Given $S_1 = s_1, S_2 = s_2, ..., S_k = s_k$

Under the null hypothesis $H_0 : \Delta = 0$, W is distributed conditionally as a sum of independent random variables $x_{i1}, i = 1, 2, ..., k$ each having a hyper geometric distribution,

$$f_i(x|0, s_i) = \frac{\binom{n_{i1}}{x}\binom{n_{i2}}{s_i - x}}{\binom{n_{i1} + n_{i2}}{s_i}}, a_i \leq x \leq b_i.$$

Thus, $E_{H_0}(x_{i1}|s_i) = s_i\left(\frac{n_{i1}}{n_i}\right)$ where $n_i = n_{i1} + n_{i2}$.

$$v_i = Var_{H_0}(x_i|s_i) = \frac{n_{i1}n_{i2}s_i(n_i - s_i)}{n_i^2(n_i - 1)}.$$

The Mantel-Hanszel statistic is

$$\chi_1^2 = \frac{[|\sum_{i=1}^{k} x_{i1} - \sum_{i=1}^{k} E_{H_0}(x_{i1})| - 0.50]^2}{\sum_{i=1}^{k} v_i}.$$

Equivalent Form of the Mantel-Hanszel Statistic

Let $w_i = \frac{n_{i1}n_{i2}}{n_{i1}+n_{i2}}, i = 1, 2, ..., k \ p_{i1} = \frac{x_{i1}}{n_{i1}}, p_{i2} = \frac{x_{i2}}{n_{i2}}, n_i = n_{i1} + n_{i2}, \bar{p}_i = \frac{x_{i1}+x_{i2}}{n_{i1}+n_{i2}}$. $\bar{p}_i$ is a pooled estimate of a common value of θ_{i1} and θ_{i2} under H_0. Then the Mantel-Hanszel statistic is also given by

$$\chi_1^2 = \frac{(|\sum_{i=1}^k w_i(p_{i1} - p_{i2})| - 0.50)^2}{\sum_{i=1}^k \frac{n_i w_i \bar{p}_i(1-\bar{p}_i)}{n_i - 1}}.$$

This form of the statistic is appealing because of its similarity to the statistic used to compare two independent binomial proportions.

Rule of Five

Mantel and Hanszel suggested the following rule for deciding when the sample sizes (or number of groups) is large enough to adequately approximate the null distribution of their χ^2 statistic by the chi-square distribution. $\sum_{i=1}^k E_i - \sum_{i=1}^k L_i > 5$ and $\sum_{i=1}^k H_i - \sum_{i=1}^k E_i > 5$ where $E_i = n_{i1}\bar{p}_i, M_i = n_i\bar{p}_i, L_i = \max(0, M_i - n_{i2}), H_i = \min(n_{i1}, M_i)$.

Example: To study a new drug for hypertension (Fleiss, 1986), a total of $n = 41$ patients were available who had recently experienced a stroke. Of these, 16 were given the new drug and the remaining 25 served as a control. The patients were grouped by age. x_{ij} is the number of patients not experiencing a new stroke during a certain recovery period.

Age Strata	1 (Drug)	2 (Control)
1	$x_{11} = 4$	$x_{12} = 0$
	$n_{11} = 4$	$n_{12} = 1$
2	$x_{21} = 7$	$x_{22} = 3$
	$n_{21} = 11$	$n_{22} = 11$
3	$x_{31} = 1$	$x_{32} = 4$
	$n_{31} = 1$	$n_{32} = 13$

The analysis can be done in terms of 2×2 tables.

Strtm	Trt	No Strk	Strk		x_{i1}	M_{i1}	V_i
1	1	4	0	4	4	$\frac{4(4)}{5} = 3.2$	$\frac{4(1)(4)(1)}{5^2(4)} = 0.16$
	2	0	1	1			
		4	1	5			
2	1	7	4	11	7	$\frac{10(11)}{22} = 5.0$	$\frac{10(12)(11)(11)}{(22)^2(21)} = 1.43$
	2	3	8	11			
		10	12	22			
3	1	1	0	1	1	$\frac{5(1)}{14} = 0.36$	$\frac{5(9)(1)(13)}{(14)^2(13)} = 0.23$
	2	4	9	13			
		5	9	14			

$\sum x_{i1} = 4 + 7 + 1 = 12, \sum M_{i1} = 8.56, \sum V_i = 1.82$. The hypotheses are $H_0 : \Delta = 0$, versus $H_1 : \Delta \neq 0$. $\chi^2_{obs} = \frac{(|\sum x_{i1} - \sum M_{i1}| - 0.50)^2}{\sum V_i} = 4.75$, $\alpha = 0.05$. Since $\chi^2_{obs} > 3.841$, reject the null hypothesis. The Mantel-Hanszel statistic is not appropriate if there is evidence of interaction. In particular, the direction of the treatment effect should tend to be constant across strata.

Check of the Adequacy of the χ^2 Approximation

Strm	Trt 1	Trt 2	n_i	$\bar{p}_i$	E_i	M_i	L_i	H_i
1	$x_{11} = 4$	$x_{12} = 0$						
	$n_{11} = 4$	$n_{12} = 1$	5	0.80	3.2	4.0	3	4
2	$x_{21} = 7$	$x_{22} = 3$						
	$n_{21} = 11$	$n_{22} = 11$	22	0.45	4.95	9.9	0	9.9
3	$x_{31} = 1$	$x_{32} = 4$						
	$n_{31} = 1$	$n_{32} = 13$	14	0.36	0.36	5.04	0	1.0

$\sum E_i = 8.51, \sum L_i = 3, \sum E_i - \sum L_i = 8.51 - 3 = 5.51 > 5$. $\sum H_i = 14.9, \sum H_i - \sum E_i = 6.39 > 5$. The sample sizes barely satisfy the rule of five.

12.15 Summary of Peto, et. al. (1976) Part I

Section 3. Numbers of patients required.

- The ability of a trial to distinguish between two treatments depend upon how many patients die rather than on the number of patients entered.
- Clinical trials about the influence of treatment on time to death should rarely be undertaken unless: a) there is some home that the death rate can be halved, or b) the trial will be able to continue until at least 100 patients have died.

Section 4. What treatment schedules should be compared?

- The question to be answered by a clinical trial should be the most important question the investigators can think of.
- A lesser study of an important question is usually of more value than an excellent study of a trivial question.
- Many trials yield null results and it is a mark of a good trial design that a null result, if it occurs, will be of interest.
- If you are trying out a new drug, give the biggest dose of it you safely can so nobody can say, if you get a negative result, that if only you had given more, it would have worked.
- A drug trial is always a trial of the drug in the particular dose and manner given, not a trial of the drug per say.
- A question is more likely to be successfully answered by a clinical trial if it can be answered by comparing just two alternative treatments and no more, those treatments being as markedly different as possible.
- The most common reason for deviations from a treatment schedule is treatment toxicity, necessitating that less than a specified dose be given or that courses of treatment be delayed.
- Specification of treatment schedules should therefore include details of what to do if undue toxicity emerges (i.e. details concerning the flexibility permitted in the treatment schedule).

Section 11. Treatment allocation.

- Balanced randomization at the latest possible time is recommended, with no stratification.
- Balanced randomization means that randomization is performed in such a way that approximately equal numbers of patients would be equally allocated to each of the treatment groups if the trial were to end earlier than scheduled.
- One reason for waiting until the latest possible moment to randomize each patient is so that almost immediately after randomization the patients in different groups will start to receive the different treatments.
- In large trials, there is no need for randomization to be stratified by some prognostic variable.
- Instead, groups of patients can be formed at the analysis stage using those features (e.g. age or disease stage) which are eventually found to be really relevant to prognosis.
- This is called post (or retrospective) stratification.
- The patients within each stratum are then compared with each other and the results combined over different strata to give an overall p-value for the effect of treatment adjusted for the grouping variable.
- The only advantage gained by stratification at entry is that reasonable balance between the numbers on each treatment will automatically be achieved and a wasteful situation where almost all patients happen to get the same treatment is avoided.
- This advantage, however, is an illusion unless the trial is very small.

Section 13. Exclusions, withdrawals, losses. This topic was discussed extensively during the first week of class.

Section 14. When to analyze and publish your results.

1. Early analysis of a trial can be misleading if a temporary difference causes the trial to be aborted so that large numbers of patients never accumulate.
2. Most statistical tests applied to clinical trial data are based on the assumption, usually false, that the decision to stop and publish has been taken independently of the current results.
3. However, it is not uncommon to examine the data say every 6 months, and if there is an apparent difference, a more formal analysis is then undertaken, the trial then stopped and the results published if a positive result is obtained.
4. Suppose the nominal significance level is 0.05 and we look at the data on 5 different occasions to determine whether the results are yet significant at the 0.05 level.
5. Then, the actual significance level is actually about 0.15 rather than the 0.05 that is claimed.
6. For this reason, many published p-values should be doubled or tripled.
7. Simple rule: Avoid any analysis or brief inspection until dozens of deaths have accumulated for it is trials first looked at when very small that are most likely to be misleading.

Section 15. Ethical considerations.

- To avoid having trials grind to a halt before obtaining statistical significance, it may be necessary to keep the treating physicians ignorant of the current state of the treatment comparison and only allow access to the trial results by the steering committee.
- If a developing trend has already been appreciated by the treating physician before his last patient is randomized, how can allocation to the inferior treatment be justified?

- A continuation of this argument suggests that serious consideration of each patient's welfare will lead to policies that prevent any clinical trial from producing a clear answer.

- However, an ethical imperative exists which is frequently ignored that we must, if we can, discover how patients can be treated most effectively; thus policies against randomization are detrimental to the very people they are intended to help.

12.16 Homework and Answers

1. A trial is conducted at two different centers to study the difference in mortality for two treatment groups. A total of 22 subjects at center 1 are randomly and equally allocated to the two treatment groups. Similarly, 20 subjects at center 2 are randomly and equally allocated to the two treatment groups. Use the data on the attached pages to do the following:

   (a) Use the combined set of trial times from both centers to construct the Kaplan-Meier estimate of the survival function for the group receiving treatment 1. Solution: The combined set of treatment #1 trial times:

Trial Time	# at Risk	# of Deaths	Interval Probability of Death	of Survival	Survival Probability $\widehat{F}(t)$
2.6	21	1	0.048	0.952	0.95
3.9	20	1	0.050	0.950	0.90
4.3	19	1	0.053	0.947	0.86
4.8	18	1	0.056	0.944	0.81
5.4	17	2	0.118	0.882	0.71
5.4					
6.9	15	1	0.067	0.933	0.67
7.8^{+}	14	0			
7.9	13	1	0.077	0.923	0.61
8.1^{+}	12	0			
8.2	11	1	0.091	0.909	0.56
8.3	10	1	0.100	0.900	0.50
10.5^{+}	9	0			
11.0^{+}	8	0			
11.2	7	1	0.143	0.857	0.43
12.2	6	1	0.167	0.833	0.36
12.3^{+}	5	0			
13.8^{+}	4	0			
14.8	3	1	0.333	0.667	0.24
16.0^{+}	2	0			
16.2^{+}	1	0			

The following table contains the combined trial times at Center #1.

Trial Time	Trt	Treatment Group 1 # at Risk	Treatment Group 1 # of Deaths	Treatment Group 2 # at Risk	Treatment Group 2 # of Deaths
3.9	1	11	1	11	0
5.4	1	10	1	11	0
6.9	1	9	1	11	0
7.7	2	8	0	11	1
7.8^+	1				
7.9	2	7	1	10	1
7.9	1				
8.2	1	6	1	9	1
8.2	2				
8.3	1	5	1	8	0
10.5	24	0	8	1	
10.5^+	1				
11.0^+	1				
12.2	2	2	0	7	1
12.5	2	2	0	6	1
14.8	1	2	1	5	0
16.0^+	1				
16.6	2	0	0	5	1
16.9^+	2				
17.1^+	2				
18.1^+	2				
19.5^+	2				

The following table contains the combined trial times at Center #2.

Trial Time	Trt	Treatment Group 1 # at Risk	Treatment Group 1 # of Deaths	Treatment Group 2 # at Risk	Treatment Group 2 # of Deaths
2.6	1	10	1	10	0
4.3	1	9	1	10	0
4.8	1	8	1	10	0
5.4	1	7	1	10	0
7.7	2	6	0	10	1
7.8	2	6	0	9	1
8.1	2	6	0	8	1
8.1^+	1				
8.2	2	5	0	7	1
10.1	2	5	0	6	1
11.2	1	5	1	5	0
12.2	1	4	1	5	0
12.3^+	1				
13.8^+	1				
14.1	2	1	0	5	1
16.2^+	1				
16.9	2	0	0	4	1
17.3^+	2				
22.1	2				
23.9^+	2				

(b) Use the adjusted (for centers) log rank statistic to test the hypothesis of no difference in survival functions for the two treatment groups. Show how you are making the calculations. Solution:

The following sets of 2×2 tables contain the adjust log rank statistic for the trial times at Center #1.

		D	S		d_{1i}	$e_i = E_{H_0}(d_{1i})$	$v_i = Var_{H_0}(d_{1i})$
$t_9 = 12.2$	1	0	2	2	0	0.22	$\frac{1(8)(2)(7)}{(9)^2(8)} = 0.17$
	2	1	6	7			
		1	8	9			
$t_{10} = 12.5$	1	0	2	2	0	0.25	$\frac{1(7)(2)(6)}{(8)^2(7)} = 0.19$
	2	1	5	6			
		1	7	8			
$t_{11} = 14.8$	1	1	1	2	1	0.29	$\frac{1(6)(2)(5)}{(7)^2(6)} = 0.20$
	2	0	5	5			
		1	6	7			
$t_{12} = 16.6$	1	0	0	0	0	0.00	$\frac{1(4)(0)(5)}{(5)^2(4)} = 0.00$
	2	1	5	6			
		1	4	5			

$D_1 = \sum d_{1i} = 7$, $E_1 = \sum e_i = 4.94$, $V_1 = \sum v_i = 2.9$. The following sets of 2×2 tables contain the adjust log rank statistic for the trial times at Center #2.

		D	S		d_{1i}	$e_i = E_{H_0}(d_{1i})$	$v_i = Var_{H_0}(d_{1i})$
$t_1 = 2.6$	1	1	9	10	1	0.50	$\frac{1(19)(10)(10)}{(20)^2(19)} = 0.25$
	2	0	10	10			
		1	19	20			
$t_2 = 4.3$	1	1	8	9	1	0.47	$\frac{1(18)(9)(10)}{(19)^2(18)} = 0.25$
	2	0	10	10			
		1	18	19			
$t_3 = 4.8$	1	1	7	8	1	0.44	$\frac{1(17)(8)(10)}{(18)^2(17)} = 0.25$
	2	0	10	10			
		1	17	18			
$t_4 = 5.4$	1	1	6	7	1	0.41	$\frac{1(16)(7)(10)}{(16)^2(15)} = 0.24$
	2	0	10	10			
		1	16	17			
$t_5 = 7.7$	1	0	6	6	0	0.38	$\frac{1(15)(6)(10)}{(16)^2(15)} = 0.23$
	2	1	9	10			
		1	15	16			
$t_6 = 7.8$	1	0	6	6	0	0.40	$\frac{1(14)(6)(9)}{(15)^2(14)} = 0.24$
	2	1	8	9			
		1	14	15			
$t_7 = 8.1$	1	0	6	6	0	0.43	$\frac{1(13)(6)(8)}{(14)^2(13)} = 0.24$
	2	1	7	8			
		1	13	14			
$t_8 = 8.2$	1	0	5	5	0	0.42	$\frac{1(11)(5)(7)}{(12)^2(11)} = 0.24$
	2	1	6	7			
		1	11	12			
$t_9 = 10.1$	1	0	5	5	0	0.45	$\frac{1(10)(5)(6)}{(11)^2(10)} = 0.25$
	2	1	5	6			
		1	10	11			
$t_{10} = 11.2$	1	1	4	5	1	0.50	$\frac{1(9)(5)(5)}{(10)^2(9)} = 0.25$
	2	0	5	5			
		1	9	10			
$t_{11} = 12.2$	1	1	3	4	1	0.44	$\frac{1(8)(4)(5)}{(9)^2(8)} = 0.25$
	2	0	5	5			

$D_2 = \sum d_{1i} = 6$, $E_2 = \sum e_i = 5.01$, $V_2 = \sum v_i = 2.83$. Then, combining the statistics, $D = D_1 + D_2 = 7 + 6 = 13$, $E = E_1 + E_2 = 4.94 + 5.01 = 9.95$, $V = V_1 + V_2 = 2.9 + 2.83 = 5.73$. H_0 : the survival distributions at Centers 1 and 2 are equal, versus H_1 : the survival distributions are not equal. The test statistic is $\chi^2 = \frac{(|D-E|-0.50)^2}{V}$. Reject H_0 if $\chi^2_{obs} \geq 3.84$. $\chi^2_{obs} = \frac{(|13-9.95|-0.50)^2}{5.73} = 1.13$. Thus, do not reject H_0.

(c) Use only the data from center 1 to give a 95% confidence limit for the relative hazard rate $\phi = \frac{\lambda_1(x)}{\lambda_2(x)}$. Solution: The confidence limits for $\ln\phi$ have the form $\frac{D_1-E_1}{V} \pm \frac{z_{\alpha/2}}{\sqrt{V}}$ where $D_1 = 7, E_1 = 4.94, V = 2.9, z_{\alpha/2} = 1.96$. So, $\frac{7-4.94}{2.9} \pm \frac{1.96}{\sqrt{2.9}}$ or 0.71 ± 1.15. The lower limit is -0.44 and the upper limit is 1.86. The 95% confidence limits for ϕ are: 1) the lower limit $e^{-0.44} = 0.64$, and 2) the upper limit $e^{1.86} = 0.42$.

2. Consider a maximum duration trial of length $T = 4$ years. Assume the following:

- All subjects enter the trial at the same point in time.
- There are no losses to follow-up other than those subjects that are alive when the trial ends.
- Survival times for the two groups have distributions with proportional hazard rates: $\bar{F}_1(t) = [\bar{F}_2(t)]^{\phi}$ where $\phi = \frac{\lambda_1(x)}{\lambda_2(x)}$.
- Subjects are randomized equally to treatment 1 (a new drug) and treatment 2 (the standard drug).

(a) How many deaths must be observed before the trial ends so a 5% level test of $H_0 : \phi = 1$ versus $H_1 : \phi \neq 1$ has a power of 0.90 at the particular alternative $\phi_1 = 0.60$? Solution: $d = 4\frac{(z_{\alpha/2}+z_\beta)^2}{[\log\phi_1]^2} = \frac{41.99}{0.2609} = 160.90$

(b) Assuming 48% of the patients receiving the standard drug will die during the 4 year period, determine the total number of subjects needed so the 5% level test has a power of 0.90. Solution: $p_2 = 0.48$, $p_1 = 1-(1-p_2)^{\phi} = 1-(1-0.48)^{0.60} = 0.32$. $p = Q_1p_1 + Q_2p_2 = \frac{p_1+p_2}{2} = \frac{0.32+0.48}{2} = 0.40$, $n = \frac{d}{p} = \frac{160.90}{0.40} = 402.25$. So, $n = 403$.

3. In Exercise # 2, suppose the subjects can be grouped as follows: a) those entering after the starting date, and b) those recruited before the starting date. Let n_A and n_B denote the numbers of subjects in each of these groups. Let us replace assumption (1) in Exercise # 2 by the following:

- Group B participants are all randomized on the trial starting date and have a maximum exposure period of length of 4.0 years.
- Group A participants enter the trial at a uniform rate over a period of length $R = 2.0$ years.
- The survival times of subjects in the two treatment groups have exponential distributions with hazard rates λ_1 and λ_2.

If only $n_B = 300$ participants have been recruited before the trial begins, how many group A participants must be recruited during an initial 2 year period so the 5% level test in Exercise # 2 has a power of 0.90? Solution: $T = 4.0, R = 2.0, \phi_1 = 0.60, p_2 = 0.48, \alpha = 0.05$. $n_Ap_A + n_Bp_B = d$ where $n_B = 300, d = 160.9, p_B = 0.40$. $p_A = \frac{p_1+p_2}{2}$ where $p_i = 1 - \frac{[e^{-\lambda_i(T-R)} - e^{-\lambda_i T}]}{\lambda_i R}, i = 1,2$ $\lambda_1 = \phi_1\lambda_2$. $0.48 = p_2 = F_2(t) = 1 - \bar{F}_2(t) \Rightarrow \bar{F}_2(t) = 0.52 \Rightarrow e^{-\lambda_2 T} = 0.52 \Rightarrow \lambda_2 = \frac{-\log 0.52}{T} = \frac{-\log 0.52}{4} \Rightarrow \lambda_2 = 0.1635$. $\lambda_1 = \phi_1\lambda_2 = 0.60(0.1635) = 0.0981$. $p_1 = 1 - \frac{[e^{-(0.0981)(4-2)} - e^{-(0.0981)(4)}]}{(0.0981)(2)} = 0.2538$, $p_2 = 1 - \frac{[e^{-(0.1635)(4-2)} - e^{-(0.1635)(4)}]}{(0.1635)(2)} = 0.3849$. $p_A = \frac{p_1+p_2}{2} = \frac{0.2538+0.3848}{2} = 0.3194$. $n_Ap_A + n_Bp_B = d \Rightarrow n_A(0.3194) + 300(0.40) = 160.9 \Rightarrow n_A = 128.05$.

12.17 Comparing Proportions Across Strata

- The subjects in a clinical trial may be grouped at the time of randomization or a the analysis stage.
- When grouping occurs at the analysis stage, it is done to take advantage of explanatory information, which may improve the power of a test for detecting a treatment difference.
- It is appropriate to group the subjects using baseline measurements, but it is not appropriate to group on the basis of outcomes (e.g. level of compliance).

Pre stratification refers to grouping data at the design state. *Post stratification* refers to grouping data after the experiment has been conducted. It's accepted practice to group data by baseline measurements, but not outcomes of the experiment.

Refer to page 31 of the Peto paper for this example. x_{ij} is the number of successes observed for the n_{ij} subjects in row i, and column j. θ_{ij} is the probability of success for the subjects in row i, and column j. Ignore the grouping by clinics. Then, $\hat{\theta}_1 = \frac{(4+2)m}{(7+5)m} = \frac{6m}{12m} = 0.5$, $\hat{\theta}_2 = \frac{(8+12)m}{(13+27)m} = \frac{20m}{40m} = 0.5$, Cannot tell the difference of the two treatments, ignoring clinics. Also, in the Peto article, $\lambda_{11} = \log\left(\frac{\theta_{11}}{1-\theta_{11}}\right) = \log\left(\frac{0.57}{1-0.57}\right) = 0.282$. Suppose we have [Peto, page 32]

	Treatment	
Row	1	2
1	μ_{11}	μ_{12}
2	μ_{21}	μ_{22}
3	μ_{31}	μ_{32}

Interaction occurs between the different rows (i.e. the $\alpha_i's$ in the handout). $\Delta_1 = \Delta_2 = \cdots = \Delta_k$ in the no interaction concept. $w = \sum_{i=1}^{k} x_{i1} \sim$ hyper geometric distribution. $E_{H_0}(x_{i1}) = s_i\left(\frac{n_{i1}}{n_i}\right)$, $Var_{H_0}(x_{i1}) = s_i\left(\frac{n_{i1}}{n_i}\right)$ which are all know numbers. Then standardizing, $Z = \frac{\left(\sum_{i=1}^{k} x_{i1}\right) - \sum_{i=1}^{k} E_{H_0}(x_{i1})}{\sqrt{\sum_{i=1}^{k} v_i}}$

12.18 Censoring

Most clinical trials are simply truncated survey designs. Unknown budget restrictions occur when planning for a large survey or census where the lead time to develop and plan for it may be many years. This may limit the number of those surveyed. Known budget restrictions may stop any follow-up operations during a survey because all the dollars budgeted have been exhausted.

Censoring may occur in a number of ways:

1. The trial terminates before the patient dies.
2. A patient dies from a cause unrelated to the disease being studied.
3. A patient moves away from the clinic.

All *censored* death times are viewed as losses to follow-up. The *survival time* x of a patient is the time from randomization until death occurs. Of course, survival time would not be observed if censoring occurs. If c is the censoring time of a subject, then the subject's trial time is $\min(x, c)$ (which ever one occurs first). It is assumed x and c are independent. In some trials, events other than death my be the primary outcome of interest. For example, the primary outcome my be the occurrence of:

- First stroke.
- Disease recurrence.
- Transplant rejection.

- Etc.

We will refer to death as the primary outcome of interest.

12.18.1 Censored Survival Times

Most trials have a maximum duration that may be defined as the termination date minus the starting date. Usually, patient entry is staggered over a time period of length $R \leq T$. Patients that enter the trial near the end of the recruitment period are more likely to be active when the trial terminates than are patients that enter early. If a patient does not die during the study period, then his exposure time (T) becomes his censoring time.

12.18.2 Survival Function and Hazard Rate

Using the notation, x as the survival time, which is a non-negative random variable. Let $f(x)$ be the pdf of x. $F(t)$ or $F(x)$ is the cdf of x. $\bar{F}(t)$ or $\bar{F}(x)$ is the survival function of x. $\lambda(x)$ or $\lambda(t)$ is the hazard rate. Using the assumption that the distribution of x is continuous with some pdf,

$$\bar{F}(t) = P(x > t) = 1 - P(x \leq t) = 1 - F(t).$$

$$P(x > t) = \int_t^\infty f(x)\, dx.$$

Two notes:

1. $\bar{F}(t) = 1 - F(t)$.
2. Since x is a non-negative random variable with a distribution of $f(x)$, the pdf $f(x) = 0, \forall x < 0$.

A typical survival function has $F(t)$ plotted on the y-axis, and t plotted on the x-axis where $\bar{F}(t) = P(x > 0) = 1$. The survival function of any continuous distribution must satisfy the following:

1. $\bar{F}(0) = 1$.
2. $\bar{F}(t)$ is non-increasing in $t \geq 0$.
3. $\lim_{t\to\infty} \bar{F}(t) = 0$.

$\bar{F}(t)$ represents the proportion of a large population of patients that survive at least t time units. The *hazard rate* of a distribution with pdf $f(x)$ and a survival function $\bar{F}(t)$ is $\lambda(x) = \frac{f(x)}{\bar{F}(t)}, x \geq 0$. $\lambda(x) \geq 0$ is always true. The hazard rate uniquely determines the distribution of the survival time.

$$\int_0^t \lambda(x)\, dx = \int_0^t \frac{f(x)}{\bar{F}(x)}\, dx = \int_0^t \frac{1}{\bar{F}(x)} \partial x$$

because $\frac{dF(x)}{dx} = f(x)$. So, $\partial F(x) = f(x)\, dx$. Integrate by substitution, $u = \bar{F}(x)$, $-dF(x) = -\, du$, $d\bar{F}(x) = -dF(X)$, and substitute back,

$$\int_1^{\bar{F}(x)} -\frac{1}{u}\, du,$$

when $x = 0$, and $u = 1$. The new limits of integration are

$$\int_{\bar{F}(x)}^{1} \frac{1}{u}\,du = \ln u\Big|_{\bar{F}(x)}^{1} = 0 - \ln \bar{F}(x) = -\ln \bar{F}(x)$$

when $x = t$, and $\bar{F}(x) = u$.

$$\Rightarrow \int_0^t \lambda(x)\,dx = -\ln \bar{F}(x).$$

Raise to the power of e,

$$e^{-\int_0^t \lambda(x)\,dx} = \bar{F}(x).$$

What functions $\lambda(x)$ can be hazard rate functions?

$$\bar{F}(\infty) = \lim_{t\to\infty} \bar{F}(x) = 0 \Rightarrow 0 = e^{-\int_0^\infty \lambda(x)\,dx} = \frac{1}{e^{\int_0^\infty \lambda(x)\,dx}} \Rightarrow \lim_{t\to\infty} \int_0^t \lambda(x)\,dx = \infty.$$

Example: $\lambda(x) = \frac{1}{x}, x \geq 0$ cannot be used as a hazard rate function. $\bar{F}(x)$ must have a finite area for all t.

Example:

$$\lambda(x) = \begin{cases} e^{\beta x}, & x \geq 0. \\ 0, & x < 0. \end{cases}$$

Select β first. This function can be used as a hazard rate function.

12.19 The Hazard Rate Function

The *hazard rate function* is defined as $\lambda(x) = \frac{f(x)}{\bar{F}(x)}$, where

$$\bar{F}(x) = P(x > t) = \int_t^\infty f(x)\,dx = e^{-\int_0^\infty \lambda(x)\,dx}.$$

$\lambda(x)$ must satisfy the following properties:

1. $\lambda(x)$ must be non-negative.
2. $\lim_{t\to\infty} \int_0^t \lambda(x)\,dx = \infty$.
3. $\int_0^t \lambda(x)\,dx$ must be finite for $t \geq 0$.

Conversely, any function $\lambda(x)$ that satisfies (1) thru (3) uniquely determines a *survival function* thru the relation

$$\bar{F}(x) = e^{-\int_0^t \lambda(x)\,dx}.$$

We want $\lim_{t\to\infty} \bar{F}(x) = 0$, and $\frac{1}{e^{\int_0^t \lambda(x)\,dx}} \to 0$.

Suppose that $\int_0^t \lambda(x)\,dx = \infty \Rightarrow \bar{F}(x) = 0$ for some $t > 0 \Rightarrow \bar{F}(x) = 0$ for every $t > 0 \Rightarrow$ no one survives.

Example: $\lambda(x) = \frac{1}{x}, x > 0$. Plot x on the x-axis and $\lambda(x)$ on the y-axis.

$$\int_0^t \lambda(x)\,dx = \int_0^t \frac{1}{x}\,dx = \ln x \Big|_0^t = \ln t - \lim_{x\to\infty} \ln x \to \infty \Rightarrow \bar{F}(x) = 0$$

for every $t > 0$.

Example: Let x have an exponential distribution with pdf

$$f(x) = \begin{cases} \lambda e^{-\lambda x}, & x \geq 0. \\ 0, & \text{otherwise.} \end{cases}$$

where λ is a positive parameter. Determine (a) the survival function, and (b) the hazard rate. For (a):

$$\bar{F}(t) = \int_t^\infty f(x)\,dx = \begin{cases} 1, & \text{if } t < 0. \\ e^{-\lambda t}, & \text{if } t \geq 0. \end{cases}$$

because,

$$\int_t^\infty f(x)\,dx = \int_t^\infty \lambda e^{-\lambda x}\,dx = -e^{-\lambda x}\Big|_t^\infty = 0 - (-e^{-\lambda t}) = e^{-\lambda t}, t \geq 0.$$

For part (b):

$$\lambda(x) = \frac{f(x)}{\bar{F}(x)} = \frac{\lambda e^{-\lambda x}}{e^{-\lambda x}} = \begin{cases} \lambda, & \text{if } x \geq 0. \\ 0, & \text{if } x > 0. \end{cases}$$

Example: Let x have the pdf of a Weibull distribution $\lambda\beta x^{\beta-1}e^{-\lambda x^\beta}, x \geq 0$, where the parameters $\lambda, \beta > 0$.

$$\bar{F}(t) = \int_t^\infty f(x)\,dx = \int_t^\infty \lambda\beta x^{\beta-1}e^{-\lambda x^\beta}\,dx,$$

$$\frac{d(\lambda x^\beta)}{dx} = \lambda\beta x^{\beta-1}.$$

Using integration by parts, let $u = \lambda x^\beta$, and $du = \lambda\beta x^{\beta-1}\,dx$. Then,

$$\int_{\lambda t^\beta}^\infty e^{-u}\,du = -e^{-u}\Big|_{\lambda t^\beta}^\infty = e^{-\lambda t^\beta} = e^{-\lambda t^\beta}, t \geq 0.$$

To find the hazard function,

$$\lambda(x) = \frac{f(x)}{\bar{F}(x)} = \frac{\lambda\beta x^{\beta-1}e^{-\lambda x^\beta}}{e^{-\lambda t^\beta}} = \lambda\beta x^{\beta-1}$$

which still depends on whether or not $\beta > 1$ or if $\beta < 1$.

12.20 Estimates for $\bar{F}(t)$

To estimate $\bar{F}(t)$, there are two methods in Chapter 14 of the text book.

1. The life table method.
2. The Kaplan-Meier estimator.

Consider the empirical cdf

$$F_n(t) = \frac{\text{number of } x_i \leq t}{n} \to^D F(t) = P(x \leq t).$$

Without censoring, the two methods reduce to the theoretical cdf.

12.20.1 Life Table Method

The life table method is one of the oldest methods of estimating a survival function $\bar{F}(t)$.

- Can be used when the data is grouped into intervals and the exact failure and censoring times are not known. For example, a death may only be known to occur during a certain month.
- Requires a fairly large number of observations.
- Assumes that subjects lost to follow-up (i.e. censored) are not exposed to the risk of dying for the entire duration of the grouping interval.
- Adjusts the count of the number of individuals exposed to the risk of dying by the effective number at risk by subtracting the number of losses divided by 2, from the number of individuals alive at the beginning of the interval.

Notation:

- There are $0 = t_0 < t_1 < \cdots < t_k$ boundaries of the grouping intervals.
- d_i is the number of deaths occuring in the interval $[t_{i-1}, t_i)$.
- r_i is the number of individuals alive (at risk) just before interval t_{i-1}.
- l_i is the number of losses (censored observations) during interval $[t_{i-1}, t_i)$.
- r_i' is the effective number of individuals at risk at time $t_{i-1} = r_i - \frac{l_i}{2}$.

Let $p_i = P(x \geq t_i | x \geq t_{i-1})$ and $p_0 = P(x \geq 0) = 1$. Some notes:

1. $p_i = \frac{\bar{F}(t)}{\bar{F}(t_{i-1})}$
2. $\bar{F}(t_j) = \bar{F}(0) \times \frac{\bar{F}(t_1)}{\bar{F}(0)} \times \frac{\bar{F}(t_2)}{\bar{F}(t_1)} \times \cdots \times \frac{\bar{F}(t_j)}{\bar{F}(t_{j-1})} = p_0 \times p_1 \times p_2 \times \cdots \times p_j$.
3. $1 - p_i = 1 - \frac{\bar{F}(t_i)}{\bar{F}(t_{i-1})} = \frac{\bar{F}(t_{i-1})}{\bar{F}(t_{i-1})} - \frac{\bar{F}(t_i)}{\bar{F}(t_{i-1})} = \frac{\bar{F}(t_{i-1}) - \bar{F}(t_i)}{\bar{F}(t_{i-1})} = q_i$.
4. A natural and intuitive estimate of q_i is $q_i = \frac{d_i}{r_i'}$. Thus, the life table estimate of $\bar{F}(t)$ is $\prod_{i=1}^{j} \left[1 - \frac{d_i}{r_i'}\right]$
   (a) If $A = (x \geq t_i)$ and $B = (x \geq t_{i-1})$ the $A \subseteq B$.
   (b) $P(A|B) = \frac{P(A \cap B)}{P(B)} = \frac{P(x \geq t_i)}{P(x \geq t_{i-1})}$
   (c) $q_i = \frac{P(t_{i-1} \leq x \leq t_i)}{P(x \geq t_{i-1})} = \frac{\text{dying in } [t_{i-1}, t_i]}{\text{surviving past } t_{i-1}}$ Note that $p_0 = 1$ is always true. $\hat{q}_i = \frac{d_i}{r_i'} \Rightarrow 1 - p_i = q_i$,
   $\Rightarrow p_i = 1 - q_i$, $\Rightarrow \hat{\bar{F}}(t_j) = \hat{p}_1 \times \hat{p}_2 \times \cdots \times \hat{p}_j = (1 - \hat{q}_1)(1 - \hat{q}_2) \cdots (1 - \hat{q}_j)$.
   Since $\hat{p}_i = 1 - \hat{q}_i = 1 - \frac{d_i}{r_i'}$, $\Rightarrow \left(1 - \frac{d_1}{r_1'}\right)\left(1 - \frac{d_2}{r_2'}\right) \cdots \left(1 - \frac{d_j}{r_j'}\right) = \hat{\bar{F}}(t_j)$.

Example: The survival and censoring times of $n = 356$ subjects are grouped into one year intervals as shown in the four columns below.

Interval	r_i	d_i	l_i
0-1	356	60	0
1-2	296	47	1
2-3	248	29	5
3-4	214	24	45
4-5	145	11	63
5-6	71	4	57

Note that $q_1 = \frac{60}{356} = 0.1685$. The following table of probabilities is calculated in a similar way.

Interval	r'_i	Death $\hat{q}_i$	Survival $\hat{p}_i$	Survival $\hat{\bar{F}}(t_i)$
0-1	356	0.1685	0.8315	0.8315
1-2	295.5	0.1591	0.8409	0.6992
2-3	245.5	0.1181	0.8819	0.6166
3-4	191.5	0.1253	0.8747	0.5394
4-5	113.5	0.0969	0.9031	0.4871
5-6	42.5	0.0941	0.9059	0.4413

12.21 Proportional Hazard Rate Model

Consider two treatment groups. Let $\bar{F}_i(x)$ be the survival function for subjects in group $i = 1, 2$. Let $\lambda_i(x)$ be the hazard rate for group i. Then,

$$\bar{F}_i(t) = e^{-\int_0^t \lambda_i(x)\,dx}, i = 1, 2.$$

The proportional hazard rate model is defined by the requirement that

$$\frac{\lambda_1(x)}{\lambda_2(x)} = \phi, \forall x \geq 0, \text{ where } \phi > 0.$$

The model implies that $\lambda_1(x) = \phi\lambda_2(x), \forall x$, which implies that

$$\int_0^t \lambda_1(x)\,dx = \phi \int_0^t \lambda_2(x)\,dx$$

which implies that

$$e^{-\int_0^t \lambda_1(x)\,dx} = e^{-\phi\int_0^t \lambda_2(x)\,dx} = \bar{F}_1(t) = [\bar{F}_2(t)]^{\phi}$$

The model is robust in the sense that it does not specify a particular form of $\bar{F}_1(t)$ and $\bar{F}_2(t)$. However, the model does specify how the survival functions are related, namely $\bar{F}_1(t) = [\bar{F}_2(t)]^{\phi}, \forall t$. Similarly, the model does not specify a particular form of the hazard rates, but does specify how they are related.

Example: Which of the following pairs of hazard rates are proportional?

a. $\lambda_1(x) = \alpha_j \lambda_2(x) = \beta$.

b. $\lambda_1(x) = \alpha x^2; \lambda_2(x) = \beta x^2$.

b. $\lambda_1(x) = \alpha x^2; \lambda_2(x) = \beta x^3$.

Answers (a) and (b) only are true. Answer (c) is not a proportional constant. We say that

1. x is *stochastically* larger than y, if, $P(X > t) \geq P(Y > t), \forall t$ with strict inequality for some t.

2. x is stochastically equal to y, if, X and Y have identical distributions.

3. x is stochastically smaller then y, if, $P(X > t) < P(Y > t), \forall t$ with strict inequality for some t.

Recall that the proportional hazard rate, $\bar{F}_1(t) = [\bar{F}_2(t)]^{\phi}$, implies the following properties:

1. When $\phi = 1 \Leftrightarrow \bar{F}_1(t) = \bar{F}_2(t), \forall t$ where $x \sim F_1$ and $y \sim F_2$.

2. When $\phi > 1 \Leftrightarrow \bar{F}_1(t) < \bar{F}_2(t), \forall t$.

3. When $\phi < 1 \Leftrightarrow \bar{F}_1(t) > \bar{F}_2(t), \forall t$.

Recall from the literature that $\lambda_i(x)$ are the death rates, $\phi = \frac{\lambda_1(x)}{\lambda_2(x)}$ is critical to the comparison of the two treatments, and when $\phi > 1$, it implies that treatment 2 is superior, and when $\phi < 1$, it implies that treatment 1 is superior. The log rank statistic is the same as the Mantel-Hanszel statistic applied to a series of 2×2 tables formed at each of the death times. The notation is as follows. n is the total number of trial participants. n_i is the number of trial participants allocated to treatments $i = 1, 2$. $n = n_1 + n_2$. The procedure for calculating the log rank statistic is as follow:

1. For the combined ordered set of n trials times.

2. Place censored values after the uncensored values if they are tied.

3. At each death time t_i, form the following 2×2 table:

	D	S	
1	d_{1i}	—	r_{1i}
2	d_{2i}	—	r_{2i}
	d_i	$r_i - d_i$	r_i

4. Determine the following: $e_{1i} = E_{H_0}(d_{1i}) = d_i \frac{r_{1i}}{r_i}$, $V_i = Var_{H_0}(d_{1i}) = \frac{d_i(r_i - d_i) r_{1i} r_{2i}}{r_i^2 (r_i - 1)}$, $D_1 = \sum d_{1i}$, $E_1 = \sum e_{1i}$, $V = \sum V_i$.

where d_{1i} is the number of deaths in group 1 at time t_i. d_{2i} is the number of deaths in group 2 at time t_{2i}. $d_i = d_{1i} + d_{2i}$. r_{1i} is equal to the number of subjects alive (at risk) in group 1 just prior to time t_i. r_{2i} is equal to the number of subjects alive (at risk) in group 2 just prior to time t_i. The *log rank test* assumes that the proportional hazard rate model is the true model. In this setting, the null and alternative hypotheses are the following: H_o means there is no difference in survival distributions, and H_1 means that the two distributions differ. Alternatively stated: $H_0 : \phi = 1$, $H_1 : \phi \neq 1$. The test statistic is $\chi^2(1) = \frac{(|D_1 - E_1| - 0.50)^2}{V}$.
Reject H_0 if $\chi^2_{obs} \geq c$. The null distribution is approximately χ^2 with 1 degree of freedom. An example can be found in Peto (1977). See the handout in the next few sections.

12.21.1 The Kaplan-Meier Estimator

The Kaplan-Meier estimator is the preferred method of estimating a survival function from data obtained in a clinical trial. The actual values of the death and censoring times are known. So, there is no need to approximate the number of individuals at risk at the beginning of the intervals. The Kaplan-Meier estimator is also called the *product limit estimator*. We later show that the Kaplan-Meier estimator can be derived as a maximum likelihood estimator. The definition of the Kaplan-Meier estimator is as follow:

1. Let $t_1 < t_2 < \cdots < t_k$ denote the ordered failure (death) times.
2. The set $\{t_1, t_2, \cdots, t_k\}$ does *not* include censoring times.
3. If a failure time is tied with a censoring time, then the censored value must be placed *after* the uncensored value.
4. The failure times $t_1, t_2, \cdots, t_k$ are viewed as defining a series of grouping intervals $[t_i, t_{i+1}], i = 0, 1, ..., k$ where $t_0 = 0, t_{k+1} = \infty$ and t_0 is not a death time.
5. d_i is the number of subjects that die at time t_i.
6. m_i is the number of censored survival times in the interval $[t_i, t_{i-1})$.
7. $t_{i1}, t_{i2}, ..., t_{im_i}$ are the censored survival times in the interval $[t_i, t_{i+1})$.
8. r_i is the number of subjects at risk (still alive) just prior to t_i.
9. $r_i = (d_i + m_i) + (d_{i+1} + m_{i+1}) + \cdots + (d_k + m_k)$ which is the total number of individuals whose death or censoring time is greater or equal to t_i.
10. If $\bar{F}(t)$ is continuous, then all of the $d_i = 1$ with probability equal to 1, that is, ties do not occur.
11. However, ties will occur if survival times are recorded in discrete time unites (e.g. days).
12. Therefore, any estimate of $\bar{F}(t)$ must allow for ties. The *Kaplan-Meier estimator* is $\hat{\bar{F}}(t) = \prod_{\{i:t_i \leq t\}} \left(1 - \frac{d_i}{r_i}\right)$ which is the probability of surviving to time t.

Some notes:

- $\hat{\bar{F}}(t)$ estimates $P(x > t)$.
- The set $\{i : t_i \leq t\}$ is understood to include the case $t_0 = 0$ and the number of deaths is $d_0 = 0$.
- Thus, if $0 \leq t < t_1$, then $\hat{\bar{F}}(t) = 1 - \frac{d_0}{r_0} = 1 - 0 = 1$.
- If $t > t_k$, then $\hat{\bar{F}}(t) = \prod_{i=1}^{k} \left(1 - \frac{d_i}{r_i}\right)$. Thus $\lim_{t\to\infty} \hat{\bar{F}}(t) = \prod_{i=1}^{k} \left(1 - \frac{d_i}{r_i}\right) = 0$, which is a constant, iff $d_k = r_k = \{\text{only one person alive at } t_k\}$, iff $m_k = 0$. This is reasonable because if one or more failure times are censored after time t_k, then there is some evidence of a positive probability of surviving past time t_k.
- $\hat{\bar{F}}(t)$ is a non-increasing, right continuous step-function.

$$\hat{\bar{F}}(t) = \begin{cases} 1, & \text{if } 0 \leq t < t_1 \\ 1 - \frac{d_1}{r_1}, & \text{if } t_1 \leq t < t_2 \\ \left(1 - \frac{d_1}{r_1}\right)\left(1 - \frac{d_2}{r_2}\right), & \text{if } t_2 \leq t < t_3 \\ . & . \\ . & . \\ . & . \\ \prod_{i=1}^{k} \left(1 - \frac{d_i}{r_i}\right) & \text{if } t_k \leq t \end{cases}$$

The graph would look like:

```
-- 1|----o
    |    @-----o
    |          @-----o
    |                @-----0 etc
    |                      etc
    |
---------|-----|-----|-----|----------------- t
    0    t1    t2    t3    t4
```

Example: The ordered remission durations (in months) and censoring times of $n = 10$ subjects are the following: 3.0, 4.0^+, 5.7^+, 6.5, 6.5, 8.4^+, 10.0, 10.0^+, 12.0, 15.0 where the + represents censored times. The Kaplan-Meier estimator of survival gives the following table:

Remission	r_i	d_i	q_i	p_i	$\hat{\bar{F}}(t)$
3.0	10	1	0.1	0.9	0.9
4.0^+	9	0	0.0	1	0.9
5.7^+	8	0	0.0	1	0.9
6.5	7	2	0.285	0.714	0.643
6.5					0.643
8.4^+	5	0	0.0	1	0.482
10.0	4	1	0.25	0.75	0.482
10.0^+	—	0	0.0	1	0.482
12.0	2	1	0.50	0.50	0.241
15.0	1	1	1.0	0	0.0

There is no need to calculate the Kaplan-Meier estimator at censored survival times because $\hat{\bar{F}}(t)$ is constant over such values.

12.21.2 Examples Illustrating the Kaplan-Meier Estimator and the Log Rank Test

Here's an outline for this section.

- Estimate of survival functions for two treatment groups.
- Log-log plot for checking the proportional hazard rate assumption.
- Kaplan-Meier estimator for the combined set of trial times.
- Use of the log rank test for comparing two treatment groups.
- The adjusted log rank statistic.

12.21.3 Example (Peto, et. al., 1977)

The following example comes from the Peto article for calculating the Kaplin-Meier Estimator for treatment group 1. Note that one line in the table is used for tied ordered trial times.

Ordered Trial Times	Number at Risk r_i	Number of Deaths d_i	Interval of Death $\hat{q}_i$	Probability of Survival $\hat{p}_i$	Survival Function $\hat{\bar{F}}(t_i)$
8	12	2	0.1667	0.8333	0.8333
8					
52	10	1	0.1000	0.9000	0.7500
63	9	2	0.2222	0.7778	0.5833
63					
220	7	1	0.1429	0.8571	0.5000
365^+					
852^+					
1296^+					
1328^+					
1460^+					
1976^+					

The next table shows the calculations for treatment group 2.

Ordered Trial Times	Number at Risk r_i	Number of Deaths d_i	Interval of Death $\hat{q}_i$	Probability of Survival $\hat{p}_i$	Survival Function $\hat{\bar{F}}(t_i)$
13	13	1	0.0769	0.9231	0.9231
18	12	1	0.0833	0.9167	0.8462
23	11	1	0.0909	0.9091	0.7693
70	10	1	0.1000	0.9000	0.6924
76	9	1	0.1111	0.8889	0.6154
180	8	1	0.1250	0.8750	0.5385
195	7	1	0.1429	0.8571	0.4616
210	6	1	0.1667	0.8333	0.3846
632	5	1	0.2000	0.8000	0.3077
700	4	1	0.2500	0.7500	0.2308
1296	3	1	0.3333	0.6667	0.1539
1990^+					
2240^+					

Log-Log Plot for Checking the Proportional Hazard Rate Assumption

Group 1			Group 2		
Ordered Death Times	$\hat{\bar{F}}_1(t_i)$	$-\log -\log \hat{\bar{F}}_1(t_i)$	Ordered Death Times	$\hat{\bar{F}}_2(t_i)$	$-\log -\log \hat{\bar{F}}_2(t_i)$
0	1.0000	undefined	0	1.0000	undefined
8	0.8333	1.70	13	0.9231	2.53
52	0.7500	1.25	18	0.8462	1.79
63	0.5833	0.62	23	0.7693	1.34
220	0.5000	0.37	70	0.6924	1.00
			76	0.6154	0.72
			180	0.5385	0.48
			195	0.4616	0.26
			210	0.3846	0.05
			632	0.3077	-0.16
			700	0.2308	-0.38
			1296	0.1539	-0.63

Plotting $-\log -\log \hat{\bar{F}}(t_i)$ on the y-axis and ordered death times on the x-axis, the two plots do criss-cross each other. Thus, there is a possible violation of the proportional hazard rate assumption.

12.21.4 Example Based on the Combined Data

The following table shows the calculations for the Kaplan-Meier Estimator based on the combined data for groups 1 and 2 of Peto, et. al., 1977.

Ordered Trial Times	Treatment Group	Number at Risk r_i	Number of Deaths d_i	Interval of Death $\hat{q}_i$	Probability of Survival $\hat{p}_i$	Survival Function $\bar{\hat{F}}(t_i)$
8	1	25	2	0.080	0.920	0.920
8	1					
13	2	23	1	0.043	0.957	0.880
18	2	22	1	0.045	0.955	0.840
23	2	21	1	0.048	0.952	0.800
52	1	20	1	0.050	0.950	0.760
63	1	19	2	0.105	0.895	0.680
63	1					
70	2	17	1	0.059	0.941	0.640
76	2	16	1	0.063	0.938	0.600
180	2	15	1	0.067	0.933	0.560
195	2	14	1	0.071	0.929	0.520
210	2	13	1	0.077	0.923	0.480
220	1	12	1	0.083	0.917	0.440
365^+	1	11				
632	2	10	1	0.100	0.900	0.396
700	2	9	1	0.111	0.889	0.352
852^+	1	8				
1296	2	7	1	0.143	0.857	0.302
1296^+	1					
1328^+	1	5				
1460^+	1	4				
1976^+	1	3				
1990^+	2	2				
2240^+	2	1				

12.21.5 Hypothesis Testing

This section shows the calculations using the Log Rank statistic to test the hypothesis of no difference in the survival distributions. The following table contains 15 death times. Thus, there will be 15 2×2 tables.

t_i		D	S		d_{1i}	$e_i = E_{H_0}(d_{1i})$	$v_i = Var_{H_0}(d_{1i})$
$t_1 = 8$		D	S		2	$\frac{2(12)}{25} = 0.96$	$\frac{2(23)(12)(13)}{(25)^2(25-1)} = 0.48$
	1	2	10	12			
	2	0	13	13			
		2	33	25			
$t_2 = 13$		D	S		0	$\frac{1(10)}{23} = 0.43$	$\frac{(22)(10)(13)}{(23)^2(23-1)} = 0.25$
	1	0	10	10			
	2	1	12	13			
		1	22	23			
$t_3 = 18$		D	S		0	0.45	0.25
	1	0	10	10			
	2	1	11	12			
		1	21	22			
$t_4 = 23$		D	S		0	0.48	0.25
	1	0	10	10			
	2	1	10	11			
		1	20	21			
$t_5 = 52$		D	S		1	0.50	0.25
	1	1	9	10			
	2	0	10	10			
		1	19	20			
$t_6 = 63$		D	S		2	0.95	0.47
	1	2	7	9			
	2	0	10	10			
		2	17	19			
$t_7 = 70$		D	S		0	0.41	0.24
	1	0	7	7			
	2	1	9	10			
		1	16	17			
$t_8 = 76$		D	S		0	0.44	0.25
	1	0	7	7			
	2	1	8	9			
		1	15	16			
$t_9 = 180$		D	S		0	0.47	0.25
	1	0	7	7			
	2	1	7	8			
		1	14	15			
$t_{10} = 195$		D	S		0	0.50	0.25
	1	0	7	7			
	2	1	6	7			
		1	13	14			
$t_{11} = 210$		D	S		0	0.54	0.25
	1	0	7	7			
	2	1	5	6			
		1	12	13			
$t_{12} = 220$		D	S		1	0.58	0.24

Note that $D_1 = \sum d_{1i} = 6$, $E_1 = \sum e_{1i} = 8.34$, $V = \sum v_i = 4.17$, $\chi^2_{obs} = \frac{(|D_1 - E_1| - 0.50)^2}{V} = \frac{(|16 - 8.34| - 0.50)^2}{4.17} = 0.81$. Peto, et al (1977) give a different value of χ^2. This is primarily because they did not use the continuity correction factor.

12.21.6 Adjusted Log Rank Statistic

The following section covers a test of no significance in survival distributions from the previous section. Use the following legend. 'N = Normal', 'I = Impaired.' The procedure is as follow:

1. Group the trial times by Renal Function.
2. Calculate D_{1i}, E_{1i}, and V_{1i}, for stratum $i = 1, 2$.
3. Determine $D = D_1 + D_2$, $E = E_1 + E_2$, $V = V_1 + V_2$, and $\chi^2 = \frac{(|D-E|-0.50)^2}{V}$ with one degree of freedom.

12.21.7 Adjusted Log Rank Statistic

The survival distribution of a population of patients may depend on some explanatory variable. For example, blood pressure, gender, heart rate, etc may affect a patient's survival time. If patients are grouped by different levels of some explanatory variable, then patients with-in groups may be more homogeneous with respect to the survival time than the group as a whole. Adjusting the log rank statistic by grouping on the basis of an explanatory variable often gives a more sensitive test or a treatment effect. We use the example of Peto, et al to show the effect of grouping.

The $n = 25$ patients were classified at baseline as having normal (N) or impaired (I) renal kidney function. Our previous analysis of this data indicated no difference in survival distributions for the two treatment groups when testing at $\alpha = 0.05$. This analysis however ignored the possible effect on survival of a good or poor prognosis. What kinds of measurements can be used as a basis for grouping the data and using the adjusted log rank statistic? There is nearly universal agreement that any baseline measure (i.e. pre-randomization) can be used as an explanatory variable. This would include age, gender, good/poor prognosis, high/low blood pressure, etc. Measurements taken after randomization are generally viewed as outcomes and not appropriate as explanatory variables.

Consider the regression model for two treatment groups $y = \alpha + \beta x + \epsilon$ for the pairs $(x_i, y_i), i = 1, 2, ..., n_1$, and the pairs $(x_i, y_i), i = 1, 2, ..., n_2$. The model can be re-written as $y = \beta x + \delta z + \epsilon$, for $z = 1$ for group 1, and for $z = 2$ for group 2. The hypotheses of interest are $H_0 : \delta = 0$, versus $H_1 : \delta \neq 0$. The procedure is as follow:

1. Group the trial times by renal function.
2. Calculate D_{1i}, E_{1i}, V_{1i} for strata $i = 1, 2$.
3. Determine $D = D_1 + D_2, E = E_1 + E_2$, and $V = V_1 + V_2$ and $\chi^2 = \frac{(|D-E|-0.50)^2}{V}$ with 1 degree of freedom.

Ordered Trial Times	Treatment Group	Renal Kidney Function
8	1	I
8	1	N
13	2	I
18	2	I
23	2	I
52	1	I
63	1	I
63	1	I
70	2	N
76	2	N
180	2	N
195	2	N
210	2	N
220	1	N
365^+	1	N
632	2	N
700	2	N
852^+	1	N
1296	2	N
1296^+	1	N
1328^+	1	N
1460^+	1	N
1976^+	1	N
1990^+	2	N
2240^+	2	N

Trial Times of the Impaired Group

Ordered Trial Times	Treatment Group	Treatment Group 1		Treatment Group 2	
		No. at Risk	No. Deaths	No. at Risk	No. Deaths
8	1	4	1	3	0
13	2	3	0	3	1
18	2	3	0	2	1
23	2	3	0	1	1
52	1	3	1	0	0
63	1	2	2	0	0
63	1				

t_i					d_{1i}	$e_i = E_{H_0}(d_{1i})$	$v_i = Var_{H_0}(d_{1i})$
$t_1 = 8$		D	S		1	0.57	$\frac{1(6)(4)(3)}{(17)^2(6)} = 0.24$
	1	1	3	4			
	2	0	3	3			
		1	6	7			
$t_2 = 13$		D	S		0	0.50	$\frac{1(5)(3)(3)}{(6)^2(5)} = 0.25$
	1	0	3	3			
	2	1	2	3			
		1	5	6			
$t_3 = 18$		D	S		0	0.60	$\frac{1(4)(3)(2)}{(5)^2(4)} = 0.24$
	1	0	3	3			
	2	1	1	2			
		1	4	5			
$t_4 = 23$		D	S		0	0.75	$\frac{1(3)(3)(1)}{(4)^2(3)} = 0.19$
	1	0	3	3			
	2	1	0	1			
		1	3	4			
$t_5 = 52$		D	S		1	1	$\frac{1(2)(3)(0)}{(3)^2(2)} = 0$
	1	1	2	3			
	2	0	0	0			
		1	2	3			
$t_6 = 63$		D	S		2	2	$\frac{1(1)(2)(0)}{(2)^2(1)} = 0$
	1	2	0	2			
	2	0	0	0			
		2	0	2			

Then, $D_1 = \sum d_{1i} = 4$, $E_1 = \sum e_i = 5.42$, and $V = \sum v_i = 0.92$.

Trial Times of the Normal Renal Group

Ordered Trial Times	Treatment Group	Treatment Group 1		Treatment Group 2	
		No. at Risk	No. Deaths	No. at Risk	No. Deaths
8	1	8	1	10	0
70	2	7	0	10	1
76	2	7	0	9	1
180	2	7	0	8	1
195	2	7	0	7	1
210	2	7	0	6	1
220	1	7	1	5	0
365^+	1				
632	2	5	0	5	1
700	2	5	0	4	1
852^+	1				
1296^+	2	4	0	3	1
1328^+	1				
1460^+	1				
1976^+	1				
1990^+	2				
2240^+	2				

t_i					d_{1i}	$e_i = E_{H_0}(d_{1i})$	$v_i = Var_{H_0}(d_{1i})$
$t_1 = 8$		D	S		1	0.44	$\frac{1(17)(10)(8))}{(18)^2(17)} = 0.25$
	1	1	7	8			
	2	0	10	10			
		1	17	18			
$t_2 = 70$		D	S		0	0.41	$\frac{1(16)(7)(10)}{(17)^2(16)} = 0.24$
	1	0	7	7			
	2	1	9	10			
		1	16	17			
$t_3 = 76$		D	S		0	0.44	$\frac{1(15)(7)(9)}{(16)^2(15)} = 0.25$
	1	0	7	7			
	2	1	8	9			
		1	15	16			
$t_4 = 180$		D	S		0	0.47	$\frac{1(14)(7)(8)}{(15)^2(14)} = 0.25$
	1	0	7	7			
	2	1	7	8			
		1	14	15			
$t_5 = 195$		D	S		0	0.50	$\frac{1(13)(7)(7)}{(14)^2(13)} = 0.25$
	1	0	7	7			
	2	1	6	7			
		1	13	14			
$t_6 = 210$		D	S		0	0.54	$\frac{1(12)(7)(6)}{(13)^2(12)} = 0.25$
	1	0	7	7			
	2	1	5	6			
		1	12	13			
$t_7 = 220$		D	S		1	0.58	$\frac{1(11)(5)(7)}{(12)^2(11)} = 0.24$
	1	1	6	7			
	2	0	5	5			
		1	11	12			
$t_8 = 632$		D	S		0	0.50	$\frac{1(9)(5)(5)}{(10)^2(9)} = 0.25$
	1	0	5	5			
	2	1	4	5			
		1	9	10			
$t_9 = 700$		D	S		0	0.56	$\frac{1(8)(5)(4)}{(9)^2(8)} = 0.25$
	1	0	5	5			
	2	1	3	4			
		1	8	9			
$t_{10} = 1296$		D	S		0	0.57	$\frac{1(6)(4)(3)}{(7)^2(6)} = 0.24$
	1	0	4	4			
	2	1	2	3			
		1	6	7			

Then, $D_1 = \sum d_{1i} = 2$, $E_1 = \sum e_i = 5.01$, and $V = \sum v_i = 2.47$.

Summary for the Adjusted Log Rank Statistic Example

$D = D_1 + D_2 = 4 + 2 = 6$, $E = E_1 + E_2 = 5.42 + 5.01 = 10.43$, $V = V_1 + V_2 = 0.92 + 2.47 = 3.39$, $\chi^2_{obs} = \frac{(|D-E|-0.50)^2}{V} = 4.55$. For $\alpha = 0.05$, reject H_0 if $\chi^2_{obs} \geq 3.84$. Thus, reject H_0.

12.22 Asymptotic Distribution of the Log Rank Statistic

Let $Z = \frac{D_1 - E_1}{\sqrt{V}}$, where D_1, E_1, and V were defined earlier under the proportional hazard rate model and the assumption that the survival times have a continuous distribution. It has been shown that (Biometrika, Schoenfeld, 1981, p316) that Z has an approximate limiting Normal distribution with a variance of 1. Let the mean, $\mu = (\log\phi)\sqrt{Q_1 Q_2 np}$ where $Q_i = \frac{n_i}{n}, i = 1, 2$, $\phi = \frac{\lambda_1(x)}{\lambda_2(x)}, x \geq 0$, p is the population proportion of subjects in the combined treatment groups that die before the trial ends which is $Q_1 p_1 + Q_2 p_2$ where p_i is the proportion in group i that die before the trial ends and $n = n_1 + n_2$. The log rank test for one sided alternatives is as follow. Consider the problem of testing H_0 : no difference in survival distributions for groups 1 and 2, versus H_1 : treatment 1 increases survival time relative to treatment 2. We express these hypotheses in terms of $\phi = \frac{\lambda_1(x)}{\lambda_2(x)}$ which is the death rate in group 1 divided by the death rate in group 2. So the hypotheses can be restated as $H_0 : \phi = 1$, versus $H_1 : \phi < 1$ for the test statistic $Z = \frac{D_1 - E_1}{\sqrt{V}}$. Since $\log\phi$ gives a negative number, and $E(z) = \log\phi\sqrt{Q_1 Q_2 np}$, then the implied the rejection region is $z_{obs} < z_\alpha$. If H_0 is true then $\phi = 1$ which implies that $\mu = E(z) = 0$, and z has a standard normal distribution.

12.22.1 Confidence Limits for the Relative Hazard Rate Model

The following is implied by the asymptotic result given by Schoenfeld (1981). $z' = z - (\log\phi)\sqrt{V}$ has an approximate standard normal distribution where $Z = \frac{D_1 - E_1}{\sqrt{V}}$.
On page 241 of the text book, the confidence limits for $\log\phi$ can be found. Choose the limit $z_{\alpha/2}$ from the table for the normal distribution so that

$$P\left(-z_{\alpha/2} < z < z_{\alpha/2}\right) = 1 - \alpha.$$

$$P\left(-z_{\alpha/2} < z - \log\phi\sqrt{V} < z_{\alpha/2}\right) = P\left(-z_{\alpha/2} - z < -\log\phi\sqrt{V} < z_{\alpha/2} - z\right) =$$

$$P\left(\frac{-z_{\alpha/2} - z}{\sqrt{V}} < -\log\phi < \frac{z_{\alpha/2} - z}{\sqrt{V}}\right) = P\left(\frac{z - z_{\alpha/2}}{\sqrt{V}} < \log\phi < \frac{z + z_{\alpha/2}}{\sqrt{V}}\right) =$$

On pages 7-9 of Peto, et al, for the unadjusted log rank statistic, $n = 25$, $n_1 = 12, n_2 = 13, D_1 = 6, E_1 = 8.34, V = 4.17$. The 95% confidence interval implies:

$$\frac{z}{\sqrt{V}} \pm \frac{z_{\alpha/2}}{\sqrt{V}} \Rightarrow \frac{D_1 - E_1}{V} \pm \frac{z_{\alpha/2}}{\sqrt{V}} \Rightarrow \frac{6 - 8.34}{4.17} \pm \frac{1.96}{\sqrt{4.17}} \Rightarrow (-0.56 \pm 0.96)$$

or $-1.52 < \log\phi < 0.40$ for the hazard rate $e^{-1.52} < \phi < e^{0.40}$. For $H_0 : \phi = 1$, versus $H_1 : \phi \neq 1$, $\frac{D_1 - E_1}{V}$ is the point estimate of $\log\phi \Rightarrow \log\widehat{\phi} = \frac{D_1 - E_1}{V}$ but is not usually estimated this way.

12.23 Sample Size and the Power of the Log Rank Test

Consider the problem of testing for no differences in survival distributions, $H_0 : \phi = 1$ and $H_1 : \phi < 1$ where the death rate in group 1 is less than that in group 2. Recall that $\phi = \frac{\lambda_1(x)}{\lambda_2(x)}$ and the test statistic is $z = \frac{D_1 - E_1}{\sqrt{V}}$. Reject H_0 if $z_{obs} < -z_\alpha$. Recall that the general sample size-power equation is $|\mu_1 - \mu_0| = z_\alpha \sigma_{0n} + z_\beta \sigma_{1n}$ where z_α is replaced by $z_{\alpha/2}$ for a 2 sided alternative. Recall from Schoenfeld (1981) that z has an approximate normal distribution with a variance equal to 1 as $n \to \infty$, and $\mu = \log \phi \sqrt{Q_1 Q_2 np}$. In Part I of the Peto paper, the sensitivity of the log rank test is similar, but does not give the calculation. $\mu_1 = E_{H_1}(z) = \log \phi_1 \sqrt{Q_1 Q_2 np}$, where $Q_i = \frac{n_i}{n}$, $\mu_0 = E_{H_0}(z) = 0$, $\sigma^2_{0n} = Var_{H_0}(z) = 1$, $\sigma^2_{1n} = Var_{H_1}(z) = 1$.
Then by substitution, $|\log \phi_1 \sqrt{Q_1 Q_2 np}| = z_\alpha + z_\beta$ where ϕ_1 is a particular alternative hypothesis for which a high statistical power is desired. Let p_i be the proportion of patients dying in group i before their trial time ends. And let $\theta = np$ be the combined expected number of deaths occuring before4 the trial ends. Then, the above equation can be re-written as $|\log \phi_1| \sqrt{Q_1 Q_2 \theta} = z_\alpha + z_\beta$ where $\theta = \frac{(z_\alpha + z_\beta)}{(\log \phi_1)^0 Q_1 Q_2}$.
Assuming equal allocation of subjects to the two treatment groups, we have $Q_1 = Q_2 = \frac{1}{2}$, and $d = \frac{4(z_\alpha + z_\beta)^2}{(\log \phi_1)^2}$.
To summarize the literature so far, we need to determine the sample size $n = n_1 + n_2$, needed, so that an α level, for a one sided test has the statistical power of $1 - \beta$ at a particular alternative ϕ_1. We first solve for d, then solve for n by using $n = \frac{d}{p}$. The power of the log rank test depends critically upon the expected number of deaths ($d = np$). If the probability p that a patient dies before the trial ends is quite small, then n must be quite large so that the log rank test has adequate power. According to Peto (1977), clinical trials where the time of death is of prime interest should rarely be undertaken unless either:

1. There is some hope that the death rate can be halved by the new treatment (i.e. $\phi \leq 0.50$).

2. The trial will be able to continue until at least, 100 patients have died (i.e. $d \geq 100$) which usually requires enrolling well over 100 patients.

12.24 Estimating the Proportion of Deaths Occuring in a Maximum Duration Trial

Case 1: All the subjects enter the trial at the same point in time. Assume that there are no losses due to follow-up other than those subjects who survive past the termination date. The notation is as follow. T is the trial duration. $\bar{F}_i(x)$ is the survival function of subjects in group $p_i, i = 1, 2$. $\phi = \frac{\lambda_1(x)}{\lambda_2(x)}$. p is the combined proportion of subjects who die in the interval $(0, T) = Q_1 p_1 + Q_2 p_2$. Then $p_1 = P(x \leq t) = F_1(T) = 1 - \bar{F}_1(T)$. $p_2 = P(x \leq t) = F_2(T) = 1 - \bar{F}_2(T)$. The proportional hazard rate model states that $\bar{F}_1(t) = [\bar{F}_2(t)]^\phi, \forall t \geq 0 \Rightarrow p_1 = 1 - \bar{F}_1(T) = 1 - [\bar{F}_2(T)]^\phi = 1 - (1 - p_2)^\phi$.
If treatment 2 is a standard treatment (e.g. a placebo), then p_2 can probably be estimated from a previous study or by looking in the literature.

Case 2: All the subjects are staggered entry over a time period of length R. The assumptions are as follow.

1. The entry time u of a subject is uniformly distributed over the interval $(0, R)$. That is, the pdf of U is

$$g(U) = \begin{cases} \frac{1}{R}, & \text{if } 0 \leq u \leq R. \\ 0, & \text{otherwise.} \end{cases}$$

2. The survival time X of subjects in group i has an exponential distribution with cdf

$$F_i(x) = \begin{cases} 1 - e^{-\lambda_i x}, & \text{if } x \geq 0. \\ 0, & \text{if } x < 0. \end{cases}$$

3. The relative hazard rate $F_i(x) = P(X \leq x) \Rightarrow \bar{F}_i(x) = 1 - F_i(x)$ which has the distribution

$$\bar{F}_i(x) = \begin{cases} e^{-\lambda_i x}, & \text{if } x \geq 0. \\ 1, & \text{if } x < 0. \end{cases}$$

$\phi = \frac{\lambda_1(x)}{\lambda_2(x)}$. $\bar{F}_1(x) = [\bar{F}_2(x)]^{\phi}$. $e^{-\lambda_1 x} = [e^{-\lambda_2 x}]^{\phi}$. $e^{-\lambda_1 x} = [e^{-\lambda_2 \phi x}], \forall x. \Rightarrow \lambda_1 = \lambda_2 \phi \Rightarrow \phi = \frac{\lambda_1}{\lambda_2}$, a constant in the exponential model. Let X be the survival time and $T - U$ be the patient's exposure time. p_i is the probability that a subject in group i dies during the exposure period.

$$p_i = P(X < T - U) = \int_0^R P(X \leq T - U) g(u)\, du = \int_0^R F_i(T - U) g(u)\, du = \int_0^R \frac{[1 - e^{-\lambda_i (T-U)}]}{R}\, du =$$

$$\frac{1}{R} U \bigg|_0^R - \frac{e^{-\lambda_i T}}{R} \frac{e^{\lambda_i U}}{\lambda_i} \bigg|_0^R = 1 - \frac{1}{R} \frac{e^{-\lambda_i T}}{\lambda_i} [e^{\lambda_i R} - 1] = 1 - \frac{[e^{-\lambda_i (T-R)} - e^{-\lambda_i T}]}{R \lambda_i} = p_i$$

12.25 Sample Size and Power of the Log Rank Test

Given that $\phi = \frac{\lambda_1(x)}{\lambda_2(x)}$, the hypotheses tests are $H_0 : \phi = 1$, versus $H_0 : \phi < 1$ (the death rate in group 1 is less than the death rate in group 2). The test statistic is $Z = \frac{D_1 - E_1}{\sqrt{V}}$. We reject H_0 if $z_{obs} \leq -z_\alpha$. The sample size power equation is $|\mu_1 - \mu_0| = z_\alpha \sigma_{0n} + z_\beta \sigma_{1n}$. Assuming equal allocation $Q_i = \frac{1}{2}, i = 1, 2$, the expected number of deaths is $\theta = np \Rightarrow n = \frac{\theta}{p}$.

12.25.1 Calculating p

1. Consider the case where all of the subjects enter the trial at the same point in time. Assume no losses due to follow-up other than those that survive past time T. Let p be the combined proportion of patients dying in the time interval $(0, T)$. Then, $p = Q_1 p_1 + Q_2 p_2 = \frac{p_1 + p_2}{2}$ where $p_1 = F_1(t)$, and $p_2 = F_2(t)$. Then under the PHR model $\bar{F}_1(t) = [\bar{F}_2(t)]^{\phi} \Rightarrow p_1 = (1 - p_2)^{\phi}$. Using p_2 as the standard treatment, p_2 can be guessed or estimated from a previous study.
   Example: How many deaths must be observed when a trial ends so that a 5% level test of $H_0 : \phi = 1$ versus $H_0 : \phi < 1$ has a power of 0.90 at the particular alternative $\phi_1 = \frac{1}{3}$? Solution: $\theta = \frac{4(z_\alpha + z_\beta)^2}{(\ln \phi_1)^2}, z_\alpha = 1.65, z_\beta = 1.28, \theta = \frac{4(1.65+1.28)^2}{(\ln \frac{1}{3})^2} = 208.87$.

2. Consider the case where the entry into the study over a time period of length R : 1) The entry time U has a uniform distribution over $(0, R)$, 2) the survival times have exponential distributions $\bar{F}_i(x) = e^{-\lambda_i x} \Rightarrow \phi = \frac{\lambda_1}{\lambda_2}$, and $p_i = 1 - \frac{[e^{-\lambda_i (T-R)} - e^{-\lambda_i T}]}{\lambda_i R}, i = 1, 2$.
   Example: In a trial of duration $T = 5$ years, it is estimated that 42% of the subjects receiving the standard treatment will die during the 5 year period. Assuming all subjects enter the trial at the same point in time, then determine the total number of patients n that must be randomized so that a 5% confidence level of a one-sided test has a power of 0.90. Solution: $p_2 = 0.42, \phi_1 = \frac{1}{3}, p_1 = 1 - (1 - p_2)^{\frac{1}{3}} = 1 - (1 - 0.42)^{\frac{1}{3}} = 0.17 \Rightarrow p = \frac{p_1 + p_2}{2} = \frac{0.17 + 0.42}{2} = 0.295 \Rightarrow n = \frac{\theta}{p} = \frac{208.87}{0.295} = 708.03$ or $n = 709$.

3. Consider a trial of duration of 5 years and the following two groups of subjects: Group A contains those subjects entering after the trial starting date, and Group B contains those subjects entering the trial before the starting date. Let the variables n_A be the number of group A subjects and n_B be the number of group B subjects, and $n = n_A + n_B$. The assumptions are as follow:

   (a) None of the subjects are lost to follow-up except those that live past the stopping date.
   (b) Group B participants are all randomized on the trial starting date and have a maximum exposure time of 5 years.
   (c) Group A participants enter the trial over a uniform rate of 2 years ($R = 2$).
   (d) The survival times of subjects in the two groups have exponential distributions with hazard rates λ_1, and λ_2.

   Example: If $n_B = 500$ subjects have been recruited before the trial starts, how many eligible subjects must be recruited during the 2 year period so the test in (1) has a power of 0.90? Solution: p_A is the proportion of group A subjects that die before the trial ends. p_B is the proportion of group B subjects that die before the trial ends. $p_B = 0.295$ from Question (2). We know that $n_A p_A + n_B p_B$ is the combined expected number of deaths occuring before the trial ends. Find n_A. $p_A = Q_1 p_1 + Q_2 p_2 = \frac{p_1+p_2}{2}, p_i = 1 - \frac{e^{-\lambda_i(T-R)} - e^{-\lambda_i T}}{\lambda_i R}, i = 1, 2$. We know that $R = 2, T = 5, \phi = \frac{1}{3}$. Since, $\phi = \frac{\lambda_1}{\lambda_2} \Rightarrow \lambda_1 = \phi\lambda_2$. $F_2(5) = 0.42 \Rightarrow 1 - F_2(5) = 0.58 \Rightarrow \bar{F}_2(5) = 0.58 \Rightarrow e^{-\lambda_2(5)} = 0.58, -\lambda_2(5) = \ln 0.58, \lambda_2 = 0.1089 \Rightarrow \lambda_1 = \frac{1}{3}(0.1089) = 0.0363$. $p_1 = 1 - \frac{[e^{-(0.0363)(3)} - e^{-(0.0363)(5)}]}{(0.0363)(2)} = 0.1350$. In a similar way, $p_2 = 0.3518$. Then, $p_A = \frac{p_1+p_2}{2} = \frac{0.1350+0.3518}{2} = 0.2434 \Rightarrow n_A p_A + n_B p_B = \theta \Rightarrow n_A(0.2434) + 500(0.295) = 208.87 \Rightarrow n_A = 252.11 \Rightarrow n = n_A + n_B = 253 + 500 = 753$.

12.26 Sequential Monitoring

Reference the technical report and the JAMA article for this section. A beta blocker is one of a number of drugs that can block increased sympathetic stimulation of the heart that occurs during a heart attack. These drugs decrease the oxygen demand of the heart and the susceptibility to cardiac arrythmias. The design and analysis features of the BHAT study are as follow:

- Multi-center (31 centers).
- Randomized.
- Double blinded.
- Placebo controlled trial.
- Adherence to the treatment was monitored.
- Analysis by intent to treat (page 1709 of the article).
- Sequential monitoring at calendar times 11, 16, 21, 28, 34, 40, 48 months. The trial was stopped at 40 months.
- The maximum duration of the trial was $T = 48$ months.
- The recruitment period $R = 27$ months.
- The starting date was June 19, 1978.
- 16,400 patients were recruited and checked for eligibility. Only 23% or 3,837 patients were randomized due to the following reasons: 18% could not take the study treatment, 18% already or were likely to receive the study treatment by prescription, 26% because of study design considerations, competing risks, etc, and 15% did not consent to participation.

12.26.1 Introduction

In many clinical trials, patients enter serially in time and responses to the treatment from the patients also become available serially in time. For scientific and ethical reasons, the results of the trial are reviewed periodically as they become available. Interim monitoring is now required by all trials sponsored by the NIH. Based on such monitoring, early termination of the trial may be recommended if important differences become apparent. An early decision enables switching subjects to the most beneficial treatment as was done in the BHAT study. The *multiple test of significance problem:* suppose we perform p different tests of $H_0 : \delta = 0$, versus $H_1 : \delta \neq 0$ each at the significance level α. If the tests are independent, then, overall the significance level is equal to p the probability of making a Type I error. $P(\text{test 1 rejects } H_0 \text{ or test two rejects } H_0 \text{ or } ...) = 1 - P_{H_0}(\text{all tests accept } H_0) = 1 - (1-\alpha)^p$. If $\alpha = 0.05$, then overall the significance level is $1 - (0.95)^p$ and note that $(0.95)^p \to 0$ as p increases. Thus, as p increases we become almost certain to discover a treatment effect when none exists. The following table assumes independence.

p	Overall α
2	0.0975
3	0.1427
4	0.1855
5	0.2263

12.26.2 Repeated Tests

The tests in this section are repeated based on accumulated data that are not independent. The following calculations are based on the Lan-DeMets program disk which assumes a particular form of independence. Suppose we test $H_0 : \delta = 0$ versus $H_1 : \delta \neq 0$ and each test has $\alpha = 0.05$. Reject H_0 if $|z_{obs}| \geq 1.96$. Then, this leads to the following table with an increasing p and α.

p	Overall α
2	0.07
3	0.09
4	0.11
5	0.14

12.26.3 Some Limitations

The classical methods were introduced by Wald (1947). They have not been widely used in clinical trials for the following reasons.

1. Open Design — No upper limit on the number of subjects that must be enrolled. Classical methods require that a trial continue until a decision is reached (accepted/rejected H_0).

2. The subjects must be paired; one member of each pair randomized to a new treatment group.

3. A new pair of subjects can be enrolled only after the response variable outcome is known for all previously enrolled pairs. This implies the response to the treatment must be observed over a short time period.

4. The data must be monitored continuously so that a decision can be made before enrolling the next pair.

12.26.4 Layout of the Data

Calendar Time	Treatment 1	2	Test Statistic	Accumulated Information
t_1	$n_1(t_1)$	$n_2(t_1)$	$z(t_1)$	$I(t_1)$
t_2	$n_1(t_2)$	$n_2(t_2)$	$z(t_2)$	$I(t_2)$
t_3	$n_1(t_3)$	$n_2(t_3)$	$z(t_3)$	$I(t_3)$
$\vdots$				
t_p	$n_1(t_p)$	$n_2(t_p)$	$z(t_p)$	$I(t_p)$

The information fractions are defined as $\tau(t_1), \tau(t_2), \tau(t_3), ..., \tau(t_p)$, where $\tau(t_p) = 1$. t_p is the time the trial terminates. $n_i(t)$ is the number of patients randomized to treatment i by time $t, i = 1, 2$. $n_i = n_i(t_p)$ and $n = n_1 + n_2$ is the total sample size. $z(t)$ is the standardized form of some test statistic based on the data accumulated by time t. $I(t)$ is the information accumulated by time t. $I = I(t_p)$ is the total information available when the trial is planned to terminate. $\tau(t) = \frac{I(t)}{I}, 0 \leq \tau(t) \leq 1$.

12.26.5 Information Fractions

As the calendar time passes, units of information (i.e. subjects) are collected but not necessarily at the same rate as the passing of the calendar time. For example, suppose that a trial is designed to last 4 years and recruit $n = 1,000$ subjects. If an interim analysis is conducted 2 years after the start of the trial and if a) each subject contributes one unit of information, and b) only 400 subjects have been randomized during the 2 year period, then 50% of the trial duration has passed. 40% of the total information has been collected. As implied by this example,

1. $I(t)$ is a function of the number of subjects that have entered the trial.

2. $I(t)$ is a non-decreasing function in t.

3. $\tau(t) = \frac{I(t)}{I}$ is also a non-decreasing function in t.

4. $I(t)$ is the sum of the information units contributed by individual subjects.

The term *information* also refers to information about some parameter δ contained in an estimator of $\widehat{\delta}$. The information about δ contained in $\widehat{\delta}$ is $I = \frac{1}{Var(\widehat{\delta})}$. Let $z = \frac{\widehat{\delta}-\delta}{\sqrt{Var(\widehat{\delta})}} = \sqrt{I}(\widehat{\delta} - \delta)$.

12.26.6 Sequential Monitoring of Clinical Trials

This section and sub-section considers the cases of comparing means, proportions, and survival function slopes. The notation from the previous section will be used.

Comparing Means

$\tau(t) = \frac{I(t)}{I}, \delta = \mu_1 - \mu_2, \widehat{\delta}(t) = \bar{x}_1(t) - \bar{x}_2(t)$. $Var(\widehat{\delta}(t)) = \sigma^2 \left[\frac{1}{n_1(t)} + \frac{1}{n_2(t)}\right]$, $I(t) = \frac{1}{Var(\widehat{\delta}(t))} = \frac{1}{\sigma^2\left[\frac{1}{n_1(t)} + \frac{1}{n_2(t)}\right]}$, $z(t) = \frac{\bar{x}_1(t) - \bar{x}_2(t) - \delta}{\sigma\sqrt{\left[\frac{1}{n_1(t)} + \frac{1}{n_2(t)}\right]}} = \sqrt{I(t)}\left[\widehat{\delta}(t) - \delta\right]$. $I = I(t_p) = \frac{1}{\sigma^2\left[\frac{1}{n_1} + \frac{1}{n_2}\right]}$. $\tau(t) = \frac{I(t)}{I} = \frac{\left[\frac{1}{n_1} + \frac{1}{n_2}\right]}{\left[\frac{1}{n_1(t)} + \frac{1}{n_2(t)}\right]}$. Note that equal allocation to the two groups implies that $n_1 = n_2$ and $n_1(t) = n_2(t), \forall t$. Then, $\tau(t) = \frac{\frac{2}{n_1}}{\frac{2}{n_1(t)}} = \frac{2n_1(t)}{2n_1}$

Note that $\tau(t) = \frac{n_1(t) + n_2(t)}{n_1 + n_2}$ is a common formula.

Comparing Proportions

The following notation is used for comparing proportions. $\delta = p_1 - p_2$. $\widehat{\delta}(t) = \widehat{p}_1(t) - \widehat{p}_2(t)$. $Var(\widehat{\delta}(t)) = \frac{p_1(1-p_1)}{n_1(t)} + \frac{p_2(1-p_2)}{n_2(t)}$ The hypothesis test of interest is $H_0 : p_1 = p_2 \Rightarrow p_1 = p_2 = \bar{p}$. The test statistic for testing the null hypothesis is $z = \frac{\widehat{p}_1(t)-\widehat{p}_2(t)-\delta}{\sqrt{Var_{H_0}(\widehat{\delta}(t))}}$, where $Var_{H_0}(\widehat{\delta}(t)) = \frac{\bar{p}(1-\bar{p})}{n_1(t)} + \frac{\bar{p}(1-\bar{p})}{n_2(t)}$. The information function under H_0 accumulated by time t is given by $I_0(t) = \frac{1}{Var_{H_0}(\widehat{\delta}(t))} = \frac{1}{\bar{p}(1-\bar{p})\left[\frac{1}{n_1(t)}+\frac{1}{n_2(t)}\right]}$. $\tau(t) = \frac{I_0(t)}{I}$. $I = I(t_p) = \bar{p}(1-\bar{p})\left[\frac{1}{n_1} + \frac{1}{n_2}\right]$. $\tau(t) = \frac{\frac{1}{n_1}+\frac{1}{n_2}}{\frac{1}{n_1}(t)+\frac{1}{n_2}(t)}$. Note that under equal allocation, $\tau(t) = \frac{n_1(t)+n_2(t)}{n_1+n_2}$.

Comparing Survival Distributions

$\phi = \frac{\lambda_1(x)}{\lambda_2(x)}, \forall x \geq 0$. The test statistic is $z(t) = \frac{D_1(t)-E_1(t)}{\sqrt{V(t)}}$, where D_1, E_1, and V are calculated as if the trial were terminating at time t. Recall that in the limit $(n \to \infty)$, $Var[z(t)] = 1$, and $E[z(t)] = \ln(\phi)\sqrt{Q_1(t)Q_2(t)d(t)}$ where $Q_i(t) = \frac{n_i(t)}{n_1(t)+n_2(t)}, i = 1, 2$. $I(t) = Q_1(t)Q_2(t)d(t)$. Equal allocation implies that $Q_1(t) = Q_2(t) = \frac{1}{2} \Rightarrow I(t) = \frac{d(t)}{4}$ where $d(t)$ is the expected number of deaths in the combined groups by time t. $d(t) = n \times p(t)$ where $p(t)$ is the probability of dying by time t in the combined groups. During the course of a trial, $I(t)$ is estimated by $\widehat{I}(t) = \frac{\text{observed no. deaths by time } t}{4}$. $\tau(t) = \frac{I(t)}{I}$, $I = \frac{d(t_p)}{4} \Rightarrow \tau(t) = \frac{d(t)}{d(t_p)}$. Note that we observe the number of deaths at time t but we may not have an estimate of $d(t_p)$.

Comparing Slopes

$\delta = \theta_1 - \theta_2$. $\widehat{\delta}(t)) = \widehat{\theta}_1(t) - \widehat{\theta}_2(t)$ $z = \frac{\widehat{\delta}(t))-\delta}{\sqrt{Var[\widehat{\delta}(t)]}}$, $Var[\widehat{\delta}(t))] = Var(\widehat{\theta}_1(t)) + Var(\widehat{\theta}_2(t)) = \left[\sum_{i=1}^{n_1(t)} V_{1i}^{-1}\right]^{-1} + \left[\sum_{i=1}^{n_2(t)} V_{2i}^{-1}\right]^{-1}$ where $V_{1i} = \sigma_\theta^2\left[1 + \frac{R}{S_{1i}}\right]$, and $V_{2i} = \sigma_\theta^2\left[1 + \frac{R}{S_{2i}}\right]$. Let $I_1(t) = \sum_{i=1}^{n_1(t)} V_{1i}^{-1}$ and $I_2(t) = \sum_{i=1}^{n_2(t)} V_{2i}^{-1}$ Then, $Var[\widehat{\delta}(t)] = \frac{1}{I_1(t)} + \frac{1}{I_2(t)}$. We know by definition that $I(t) = \frac{1}{Var[\widehat{\delta}(t)]}$. Let $I(t) = \left[\frac{1}{I_1(t)} + \frac{1}{I_2(t)}\right]^{-1}$. Then, $\frac{1}{I(t)} = \frac{1}{I_1(t)} + \frac{1}{I_2(t)} = Var[\widehat{\delta}(t)]$ and $\tau(t) = \frac{I(t)}{I}$ where $I = \left[\frac{1}{I_1(t_p)} + \frac{1}{I_2(t_p)}\right]^{-1}$.

12.26.7 Formulation as a Sequential Testing Problem

Let δ be a parameter representing a treatment difference. Let $z(t)$ be the test statistic. At certain selected calendar times, we wish to decide between $H_0 : \delta = 0$ versus $H_1 : \delta > 0$. A decision at time t_i requires a boundary b_i such that $z(t_i) \geq b_i \Rightarrow$ reject H_0. To determine b_i we must specify how much of the Type I error rate we wish to spend at each interim analysis. That is, we must specify $\alpha(t_1), \alpha(t_2), ..., \alpha(t_p)$ where these quantities are defined as follow:

$$\begin{aligned}
\alpha(t_1) = &\quad P_{H_0}(z(t_1) \geq b_1) \\
\alpha(t_2) = &\quad P_{H_0}(z(t_2) \geq b_2 \text{ or } z(t_1) \geq b_1) \\
\vdots & \\
\alpha(t_p) = &\quad P_{H_0}(z(t_p) \geq b_p \text{ or ... or } z(t_1) \geq b_1)
\end{aligned}$$

Notes:

1. The '*' in the articles defines a system of p equations with p unknown variables.
2. The overall significance level is $\alpha = \alpha(t_p)$.
3. $\alpha(t_i), i = 1, 2, ..., p$ is a non-decreasing sequence with an upper limit of α.
4. Specifying α alone will not uniquely determine the boundaries.

Two-Tailed Tests

When testing $H_0 : \delta = 0$ versus $H_1 : \delta \neq 0$, H_0 is rejected at time t_i if $|z(t_i)| \geq b_i$. In this case, then $\alpha(t_1) = P_{H_0}(|z(t_1)| \geq b_1), \alpha(t_2) = P_{H_0}(|z(t_1)| \geq b_1$ or $|z(t_2)| \geq b_2)$, and so on. Also, $z(t_i) \leq -b_i$ or $z(t_i) \geq b_i$). Thus the lower boundaries can be determined by symmetry from the upper boundaries and by taking α to be $\frac{\alpha}{2}$ for a two-tailed test.

12.27 Comparing Slopes in a Linear Random Effects Model with Repeated Measures

Recall that subject i visits a clinic at times $x_j, j = 1, 2, ..., L_i$. Let $L_{1i}(t)$ be the number of visits by subject i in group 1 by time t. Let $L_{2i}(t)$ be the number of visits by subject i in group 2 by time t.

$$\bar{x}_{1i}(t) = \frac{\sum_{j=1}^{L_{1i}(t)} x_j}{L_{1i}(t)},\ \bar{x}_{2i}(t) = \frac{\sum_{j=1}^{L_{2i}(t)} x_j}{L_{2i}(t)},\ S_{1i}(t) = \sum_{j=1}^{L_{1i}(t)} [x_j - \bar{x}_{1i}(t)]^2,\ S_{2i}(t) = \sum_{j=1}^{L_{2i}(t)} [x_j - \bar{x}_{2i}(t)]^2.$$

If the follow-up times are equally spaced and there are no missed visits, then these quantities vary from subject to another only because of differences in $L_{1i}(t)$ and $L_{2i}(t)$. Let the slope difference $\delta = \theta_1 - \theta_2$ be estimated by $\widehat{\delta}(t) = \widehat{\theta}_1(t) - \widehat{\theta}_2(t)$ where $\widehat{\theta}_i(t), i = 1, 2$ are estimates based on data observed by time t.

$$z(t) = \frac{\widehat{\delta}(t) - \delta}{\sqrt{Var[\widehat{\delta}(t)]}} = \sqrt{I(t)}[\widehat{\delta}(t) - \delta]$$

where

$$I(t) = \frac{1}{Var[\widehat{\delta}(t)]},\ Var[\widehat{\delta}(t)] = Var[\widehat{\theta}_1(t)] + Var[\widehat{\theta}_2(t)] = \frac{1}{\sum_{i=1}^{n_1(t)} V_{1i}^{-1} + \sum_{i=1}^{n_2(t)} V_{2i}^{-1}} = \frac{1}{I_1(t) + I_2(t)}.$$

$n_1(t)$ is the number of group 1 subjects with at least one visit. $n_2(t)$ is the number of group 2 subjects with at least one visit.

$$V_{1i} = \sigma_\theta^2[1 + R/S_{1i}],\ V_{2i} = \sigma_\theta^2[1 + R/S_{2i}],\ R = \frac{\sigma_\epsilon^2}{\sigma_\theta^2}.$$

We have

$$I(t) = \frac{1}{I_1(t) + I_2(t)}$$

where

$$I_1(t) = \sum_{i=1}^{n_1(t)} \frac{1}{\sigma_\theta^2[1 + R/S_{1i}]},\ I_2(t) = \sum_{i=1}^{n_2(t)} \frac{1}{\sigma_\theta^2[1 + R/S_{2i}]}.$$

Let $I = I(t_p)$. In general, $\tau(t) = \frac{I(t)}{I}$ does not have a simple form but it can be estimated from the data accumulated by time t. If all subjects complete all planned visits by time t_p and have the same spacings between visits, then $S_{1i} = S_{2i} = S$ and

$$I_1(t_p) = \frac{n_1}{\sigma_\theta^2[1+R/S]},\ I_2(t_p) = \frac{n_2}{\sigma_\theta^2[1+R/S]},$$

and

$$I = \frac{1}{\frac{1}{I_1(t_p)} + \frac{1}{I_2(t_p)}} = \frac{1}{\sigma_\theta^2[1+R/S]\left[\frac{1}{n_1}+\frac{1}{n_2}\right]}$$

12.28 α Spending Functions

Lan and DeMets (1983) proposed viewing $\alpha(t)$ as a function of the cumulative information fraction $\tau(t) = \frac{I(t)}{I}, 0 \le \tau(t) \le 1$. In particular, they proposed the following α spending functions:

1. $\alpha_1(\tau) = 1 - \phi(z_\alpha/\tau), 0 \le \tau \le 1$, (Obrien-Flemming)
2. $\alpha_2(\tau) = \alpha \ln[1+(e-1)/\tau], 0 \le \tau \le 1$, (Pocock).
3. $\alpha_3(\tau) = \alpha\tau^p, 0 \le \tau \le 1, p > 0$.

Each of these functions increases to α as $\tau \to 1$. The spending functions do not require specifying in advance the number or timing or the interim analyzes. The O'Brien-Flemming bounds are popular because of a low spending rate for small values of α which implies that extreme bounds initially when very little information is available. Chapter 15 of the text book show a graph of τ_i versus α. If we choose α and any one of the spending functions, then $\alpha(t_1), \alpha(t_2), ..., \alpha(t_p)$ are completely determined and it follows that the boundaries $b_1, b_2, ..., b_p$ are going to be uniquely determined. So also are the following quantities:

$$\Pi_1 = \alpha(t_1),$$

$$\Pi_2 = \alpha(t_2) - \alpha(t_1),$$

$$\vdots$$

$$\Pi_p = \alpha(t_p) - \alpha(t_{p-1}).$$

$$\alpha(t_k) = \Pi_1 + \Pi_2 + \cdots + \Pi_k.$$

We have a choice of specifying either the vector $(\Pi_1, \Pi_2, ..., \Pi_p)$ or the vector $(\alpha(t_1), \alpha(t_2), ..., \alpha(t_p)) \Rightarrow \alpha(t) = \alpha[\tau(t)], \alpha(t_p) = \alpha(1) = \alpha$. We claim that

$$\Pi_1 = P_{H_0}(z(t_1) \ge b_1),$$

$$\Pi_2 = P_{H_0}(z(t_1) < b_1 \text{ and } z(t_2) \ge b_2),$$

$$\Pi_3 = P_{H_0}(z(t_1) < b_1 \text{ and } z(t_2) < b_2 \text{ and } z(t_3) \ge b_3),$$

and so on. Proof: Let us consider only the case Π_2. Let A_1 be the event that $z(t_1) \ge b_1$, and A_2 be the event that $z(t_2) \ge b_2$. $\alpha(t_2) = P_{H_0}(A_1 \cup A_2)$, $\alpha(t_1) = P_{H_0}(A_1)$,

$$\Pi_2 = \alpha(t_2) - \alpha(t_1) = P(A_1 \cup A_2) - P(A_1) = P(A_1) + P(A_1' \cap A_2) - P(A_1) = P(A_1' \cap A_2) =$$

$$P(z(t_1) < b_1 \text{ and } z(t_2) \ge b_2),$$

$$\Pi_1 + \Pi_2 + \cdots + \Pi_p = \alpha(t_p) = \alpha.$$

12.28.1 An Approximate Solution to the Sequential Testing Problem

To determine the bounds required, we know the null distribution of $z(t_1), z(t_2), ..., z(t_p)$. The bounds can be determined approximately from the fact that as $n \to \infty$, $z(t_1), z(t_2), ..., z(t_p)$ has an approximate limiting multivariate normal pdf or equivalently that $S_i = \sqrt{\tau(t_i)}z(t_i), i = 1, 2, ..., p$ has a multivariate normal distribution. The limiting normal distribution is related to Brownian motion in the following way. $B[\tau(t)] = \sqrt{\tau(t)}z(t)$. In all of the four examples, we discussed earlier, Brownian motion gives the approximate limiting distribution. The Brownian motion (also called the Weiner process) with a drift parameter θ and a unit variance is a family of random variables $\{B(t), 0 \leq t \leq 1\}$ with the following properties:

1. $B(0) = 0$.
2. For $0 \leq S \leq t \leq 1$, $B(t) - B(S)$ has a normal distribution with a mean $E[B(t) - B(S)] = \theta(t - S)$ and a variance $Var[B(t) - B(S)] = t - S$.
3. $B(t)$ has independent increments that is for $0 = t_0 < t_1 < t_2 < \cdots < t_n = 1$. $B(t_i) - B(t_{i-1}), i = 1, 2, ..., n$ are independent.
4. $B(t)$ must be a continuous function of t.

So, some obvious questions arise. How are sequential boundaries computed? And, do the boundaries require knowing the total information function $I = I(t_p)$? Brownian motion implies $x_1 = S_1, x_2 = S_2 - S_1, ..., x_p = S_p - S_{p-1}$. Then, $B[\tau(t_i)] = \sqrt{\tau(t_i)}z(t_i)$. To calculate the mean, $x_1 = B[\tau(t_1)] = \sqrt{\tau(t_1)}z(t_1)$, $E(x_1) = \theta\tau(t_1)$, $Var(x_1) = \tau(t_1); E(x_2) = \theta[\tau(t_2) - \tau(t_1)]$, $Var(x_2) = \tau(t_2) - \tau(t_1), ..., E(x_i) = \theta[\tau(t_i) - \tau(t_{i-1})], Var(x_i) = \tau(t_i) - \tau(t_{i-1})$. Under $H_0, \delta = 0$. $E_{H_0}[z(t)] = 0$,

$$z(t) = \frac{\bar{x}_1(t) - \bar{x}_2(t) - \delta}{\sigma\sqrt{\frac{1}{n_1(t)} + \frac{1}{n_2(t)}}} \Rightarrow E_{H_0}[B[\tau(t)]] = 0$$

which corresponds to $\theta = 0$ for the drift parameter. In general, the bounds must be determined by numerical integration. The following quantities are assumed to be known.

1. $\Pi_1 = \alpha(t_1), \Pi_2 = \alpha(t_2), ...$
2. $\tau_i = \tau(t_i)$. We discussed how the bounds are computed in terms of $S_i = \sqrt{\tau(t_i)}z(t_i)$.

Suppose the exit probabilities at the first two interim analyzes are specified as $\Pi_1 = \Pi_2 = 0.01$. How do we calculate b_1 and b_2? $H_1 : \delta > 0$. Reject H_0 if $z(t_1) \geq b_1$ or $z(t_2) \geq b_2$. $\alpha(t_1) = \Pi_1, \alpha(t_2) - \alpha(t_1) = \Pi_2$. $\alpha(t_1) = 0.01$. $\alpha(t_2) = 0.02$. $\Pi_1 = 0.01 = P_{H_0}(z(t_1) \geq b_1) \Rightarrow b_1 = 2.33$. To find b_2, $\Pi_2 = 0.01 = P_{H_0}(z(t_1) < b_1 \text{ and } z(t_2) \geq b_2)$ where b_1 has already been determined. $0.01 = P_{H_0}(\sqrt{\tau(t_1)}z(t_1) < \sqrt{\tau(t_1)}b_1 \text{ and } \sqrt{\tau(t_2)}z(t_2) \geq \sqrt{\tau(t_2)}b_2) = P(S_1 < a_1 \text{ and } S_2 \geq a_2)$ where $a_1 = \sqrt{\tau(t_1)}b_1$, and $a_2 = \sqrt{\tau(t_2)}b_2$. Since a_1 is a known number, all we need to do is solve for a_2. $0.01 = P_{H_0}(x_1 < a_1 \text{ and } x_1 + x_2 > a_2)$, $H_0 \Rightarrow E_{H_0}(x_1) = E_{H_0}(x_2) = 0$ and $Var(x_1) = \tau(t_1), Var(x_2) = \tau(t_2) - \tau(t_1)$. The pdf of x_1 is

$$f_1(x_1) = \frac{1}{\sqrt{2\pi}\sigma_1} e^{-\frac{1}{2}\frac{(x_1 - \mu_1)^2}{\sigma_1^2}} = \frac{1}{\sqrt{2\pi}\sigma_1} e^{-\frac{1}{2}\frac{x_1^2}{\sigma_1^2}}, -\infty < x_1 < \infty.$$

$$f_2(x_2) = \frac{1}{\sqrt{2\pi}\sigma_2} e^{-\frac{1}{2}\frac{x_2^2}{\sigma_2^2}}, -\infty < x_2 < \infty.$$

We need to find the limits of integration from the following graph.

```
x2
|
|(0,a2)
|\ this|
| \area|
|  \   |
|   \  |   this
|    \ |   area
|     \|    too
|      \
|      |\
|      | \
|      |  \
|      |   \
-------|----\------------ x1
       a1   (a2,0)
```

We know that $x_1 + x_2 = a_2$.

$$\int_{-\infty}^{a_1}\int_{a_2-x_1}^{\infty} f_1(x_1)f_2(x_2)\,dx_2\,dx_1 = \int_{-\infty}^{a_1}\int_{a_2}^{\infty} f_1(x_1)f_2(x_2-x_1)\,dx_2\,dx_1.$$

Using integration by parts $u = x_2 - x_1$ and $du = dx_2$. Then we have

$$\int_{-\infty}^{a_1}\int_{a_2-x_1}^{\infty} f_1(x_1)f_2(u)\,du\,dx_1$$

which is identical. Changing the order of integration,

$$\int_{a_2}^{\infty}\int_{-\infty}^{a_1} f_1(x_1)f_2(x_2-x_1)\,dx_1\,dx_2 = \int_{a_2}^{\infty} h(x_2)\,dx_2$$

where

$$h(x_2) = \int_{-\infty}^{a_1} f_1(x_1)f_2(x_2-x_1)\,dx_1.$$

Do the bounds require knowing the total information $I = I(t_p)$? During the course of a trial, the total information $I = I(t_p)$ may not be known. Recall that the information fractions $\tau(t_i) = \frac{I(t_i)}{I}$ depend on I. Thus, if I is not known and interim analyzes are performed at times t_1 and t_2, say, then we cannot compute $\tau(t_1)$ and $\tau(t_2)$. Do the bounds b_1 and b_2 require that we know $\tau(t_1)$ and $\tau(t_2)$? Clearly b_1 does not depend on $\tau(t_1)$ since $\Pi_1 = P_{H_0}(z(t_1) \geq b_1)$ and $\Pi_1 = 0.01 \Rightarrow b_1 = 2.33$. Thus, the value of $\tau(t_1)$ was not used to determine b_1. Now let us consider whether b_2 depends on knowing $\tau(t_1)$ and $\tau(t_2)$. $\Pi_2 = P(z(t_1) < b_1 \text{ and } z(t_2) \geq b_2)$ where $z(t_1)$ and $z(t_2)$ have standard normal distributions but are not independent. The only way that b_2 can depend on $\tau(t_1)$ and $\tau(t_2)$ is through the covariance between $z(t_1)$ and $z(t_2)$.

THEOREM: $Cov(z(t_1), z(t_2)) = \sqrt{\frac{\tau(t_1)}{\tau(t_2)}}$ which does not depend on I because $\tau(t_1) = \frac{I(t_1)}{I}$ and $\tau(t_2) = \frac{I(t_2)}{I}$. In other words, the I term is divided-out.

12.29 Computing Boundaries and Sample Size Using LAND and GLAN

According to Roboussin, et. al. (1995), the program disk can be used to do the following:

1. Compute boundaries for a given α spending function.
2. Compute probabilities or power for given bounds.
3. Compute confidence limits.

These are options on the program disk. Reference page 16 of the technical report. However, the program disk included with the technical report seems to be an earlier version of the program. It can be used to solve (1) and (2) above, but not (3). The program disk contains two executable files LAND and GLAN. LAND can be used to solve (1) above while GLAN can be used to solve (2).

Example 1: Use the program disk to determine sequential boundaries. The boundaries are determined by the choice of

1. Spending function $\alpha^*(t)$.
2. $\alpha = \alpha^*(1)$.
3. Whether the test is one or two sided.
4. The number p of interim analyzes and the information fractions $\tau_1 < \tau_2 < \cdots < \tau_p$.

The sequential boundaries determined by using the program disk do not depend on the choice of the standardized test statistic $Z(t)$. That is, the same boundaries can be used to compare means, proportions, survival functions, and slopes. The boundaries are computed by using the program LAND and specifying items (1) through (4) listed above. The following print-out shows a LAND session.

```
Is this an interactive session? (1=yes,0=no)
1
interactive =  1
Overall significance level? (>0 and <=1)
.05
alpha = .050
One(1)- or two(2)-sided symmetric?
1
1-sided test
Use function? (1-5)
(1) OBrien-Fleming type
(2) Pocock type
(3) alpha * t
(4) alpha * t^1.5
(5) alpha * t^2
1
Use function alpha-star 1
Number of interim analyzes in the past (0 if this is the first):
2
2 pervious analyzes.
Enter times (or information fractions > 0 and < 1) in the past:
.6 .8
Previous times (or info fractions) are .6000 .8000
```

```
Time or info fraction (<= 1) of the current interim analysis?
1.0
Current time (or information fraction) is 1.000
Do you wish to input the exact or estimated information? (e.g.
number of patients or number of events, as in Lan & DeMets 89?)
(1=yes,0=no)
0
Delta will be taken to be zero.


This program generates one-sided boundaries.
n = 3
alpha =   .050
use function = 1
        Time        Bounds     alpha(i)-alpha(i-1)    cum alpha
         .60     -8.0000 2.2769        .01140           .01140
         .80     -8.0000 1.9591        .01703           .02843
        1.00     -8.0000 1.7387        .02157           .05000
```

Thus our bounds are $b_1 = 2.2769, b_2 = 1.9591, b_3 = 1.7387$.

Example 2: Use the program disk to sequentially analyze a trial. By using α spending functions, an analysis can be conducted at any time during the course of a trial while preserving the overall Type I error rate. However, the use of α spending functions requires that we estimate the cumulative information fractions $\tau(t) = \frac{I(t)}{I}$. The total information I may not be known at the time an interim analysis is desired. If bounds are based on an under-estimate of I, the result may be that we overspend α before the trial actually terminates. An example where the value of I was not known is the BHAT trial discussed in the UW Technical Report. To circumvent this problem, it has been proposed (see the Technical Report, page 12) that calendar time be used to specify the α spending rate and that cumulative information (e.g. cumulative numbers of deaths) be used to specify correlation between test statistics. The following table comes from the Beta Blocker Heart Attack trial. See page 23 of the Technical Report.

Calendar Time (Months)	Cumulative Time Fractions	Cumulative No. of Deaths $d(t)$
11	$\frac{11}{48} = 0.229$	56
16	$\frac{16}{48} = 0.250$	77
21	$\frac{21}{48} = 0.438$	126
28	$\frac{28}{48} = 0.583$	177
34	$\frac{34}{48} = 0.708$	247
40	$\frac{40}{48} = 0.833$	318
48	?	?

Example 3: Use the program disk (LAND) to enter two time scales (calendar and information) to determine sequential boundaries for a two-sided test, $\alpha = 0.05$, spending rate $\alpha^* = \alpha\tau$ (i.e. spend α by calendar time, $t_p = 48$ months).

```
Is this an interactive session? (1=yes,0=no)
1
interactive =  1
Overall significance level? (>0 and <=1)
.05
alpha = .050
One(1)- or two(2)-sided symmetric?
2
```

```
2-sided test
Use function? (1-5)
(1) OBrien-Fleming type
(2) Pocock type
(3) alpha * t
(4) alpha * t^1.5
(5) alpha * t^2
3
Use function alpha-star 3
Number of interim analyzes in the past (0 if this is the first):
5
5 pervious analyzes.
Enter times (or information fractions > 0 and < 1) in the past:
.229 .250 .438 .583 .708
Previous times (or info fractions) are .229 .250 .438 .583 .708
Time or info fraction (<= 1) of the current interim analysis?
.833
Current time (or information fraction) is .833
Do you wish to input the exact or estimated information? (e.g.
number of patients or number of events, as in Lan & DeMets 89?)
(1=yes,0=no)
1
Entering information.
Information for past analyzes:
56 77 126 177 247
Previous information 56.000 77.000 126.000 177.000 247.000
Information for current analysis:
318
Current information 318.000

Delta will be taken to be zero.


This program generates two-sided symmetric boundaries.
n = 6
alpha =   .050
use function for the lower boundary = 3
use function for the upper boundary = 3
  Time    Information       Bounds       alpha(i)-alpha(i-1)    cum alpha
  .23         56.00     -2.5287 2.5287        .01145             .01145
  .25         77.00     -2.9598 2.9598        .00105             .01250
  .44        126.00     -2.5011 2.5011        .00940             .02190
  .58        177.00     -2.4826 2.4826        .00725             .02915
  .71        247.00     -2.4988 2.4988        .00625             .03540
  .83        318.00     -2.4607 2.4607        .00625             .04165
```

Example 4: Use the program disk for study design. The power of a sequential test depends upon the timing and frequency of the interim analyzes as well as on the total number of trial participants. Examples of sample size calculations are given in the UW Technical Report (pages 5-9). To determine the sample size, we must specify the following:

1. Whether the test is one-sided or two-sided.
2. The α level and the α spending function.

3. The number of interim analyzes.
4. The information fractions.
5. The desired power.

After specifying (1) through (5), the program disk can be used to calculate the value of the drift parameter θ that gives the desired power. There are 3 ways for calculating the sample size: a) using LAND, enter the information in (1) through (4) to compute the bounds as before, b) use GLAN and the bounds obtained in step (a) to determine the value of the drift parameters θ that gives the power specified in (5); the program actually computes power for specified values of θ; thus, we must repeatedly enter different values of θ until the desired power is attained, and c) use a formula that relates sample size to the drift parameter θ to solve for n; the formula that relates sample size to θ is given in the next table.

Comparison	δ	I	n
Means	$\mu_1 - \mu_2$	$\frac{n}{4\sigma^2}$	$\frac{4\theta^2\sigma^2}{\delta^2}$
Proportions	$p_1 - p_2$	$\frac{n}{4\bar{p}(1-\bar{p})}$	$\frac{4\theta^2\bar{p}(1-\bar{p})}{\delta^2}$
Survival Functions	$\log\left[\frac{\lambda_1(x)}{\lambda_2(x)}\right]$	$\frac{d}{4}$	$n = \frac{d}{p}, d = \frac{4\theta^2}{\delta^2}$
Slopes	$\theta_1 - \theta_2$	$\frac{n}{\sigma_\theta^2[1+R/S]}$	$\frac{4\theta^2\sigma_\theta^2[1+R/S]}{\delta^2}$

Assumption: Subjects are allocated equally to the two groups. p is the probability that a subject in the combined groups dies before the trial ends. Repeated measures: $R = \sigma_\epsilon^2/\sigma_\theta^2$. Assume equal allocation, equally spaced visits, and no missed visits. Then,

$$S = \frac{Dk(k+1)}{12(k-1)},$$

where k is the number of planned visits, and D is the time between the first and last visit.

Example 5: Let the group 1 subjects receive a new drug and the group 2 subjects receive a placebo. A baseline response is observed when each subject is randomized and a final response is observed six months later. Subject accrual ends after 1.5 years. The trial duration is 2.0 years. Interim monitoring is to be done at calendar times 1.0, 1.5, and 2.0 years. The parameters are μ_i is the mean drop in cholesterol level over a 6 month period for subjects in group i, $\delta = \mu_1 - \mu_2$, and σ^2 is the common variance of 6 month changes in cholesterol levels.

a. Determine boundaries for a two-sided test with $\alpha = 0.05$, the O'Brien-Flemming spending function, and three interim analyzes, with information fractions 0.50, 0.75, and 1.00.

b. What sample size $n = n_1 + n_2$ is needed so the 5% level test in (a) has the power equal to 0.90 when $\sigma = 50$ and $\delta = 10$? Determine the value of θ accurate to the nearest hundredth of a unit.

The following interactive session with LAND solves Exercise (5a).

```
Is this an interactive session? (1=yes,0=no)
1
interactive =  1
Overall significance level? (>0 and <=1)
.05
```

```
alpha = .050
One(1)- or two(2)-sided symmetric?
2
2-sided test
Use function? (1-5)
(1) OBrien-Fleming type
(2) Pocock type
(3) alpha * t
(4) alpha * t^1.5
(5) alpha * t^2
1
Use function alpha-star 1
Number of interim analyzes in the past (0 if this is the first):
2
2 pervious analyzes.
Enter times (or information fractions > 0 and < 1) in the past:
.5 .75
Previous times (or info fractions) are .500 .750
Time or info fraction (<= 1) of the current interim analysis?
1.0
Current time (or information fraction) is 1.000
Do you wish to input the exact or estimated information? (e.g.
number of patients or number of events, as in Lan & DeMets 89?)
(1=yes,0=no)
0
Delta will be taken to be zero.


This program generates one-sided boundaries.
n = 3
alpha =   .050
use function for lower boundary = 1
use function for upper boundary = 1
        Time        Bounds     alpha(i)-alpha(i-1)    cum alpha
         .50     -2.9626 2.9626        .00305           .00305
         .75     -2.3590 2.3590        .01625           .01930
        1.00     -2.0140 2.0140        .03070           .0500
```

The upper boundaries are needed in GLAN. The GLAN session for solving Exercise (5b) is given next.

```
GLAN
Is this an interactive session? (1=yes,0=no)
1
interactive = 1
Number of interim analyzes?
3
Times of interim analyzes:
.5 .75 1.0
Analysis times: .5000 .750 1.000
Do you wish to use drift parameter (Delta) other than zero? (1=yes,0=no)
1
Enter non centrality parameter:
3.0
Delta = 3.
```

```
One(1)- or two(2) sided?
2
2-sided test
Symmetric bounds? (1=yes,0=no)
1
Two sided symmetric bounds.
Enter upper bounds in standardized form:
2.9626 2.3590 2.0140
n = 3, delta = 3.000

look    time     lower  upper    alpha(i)-alpha(i-1)    cum alpha
1        .50    -2.9626 2.9626          .20010             .20010
2        .75    -2.3590 2.3590          .39790             .59799
3       1.00    -2.0140 2.0140          .24617             .84417

Do you wish to recompute using a new drift parameter (delta) (1=yes,0=no)?
1

------------------------------
Enter new drift parameter:
3.3
Recomputing with delta = 3.3
n = 3, delta = 3.3000

look    time     lower  upper    alpha(i)-alpha(i-1)    cum alpha
1        .50    -2.9626 2.9626          .26463             .26463
2        .75    -2.3590 2.3590          .42946             .69409
3       1.00    -2.0140 2.0140          .21087             .90496

Do you wish to recompute using a new drift parameter (delta) (1=yes,0=no)?
1

------------------------------
Enter new drift parameter:
3.3
Recomputing with delta = 3.27
n = 3, delta = 3.2700

look    time     lower  upper    alpha(i)-alpha(i-1)    cum alpha
1        .50    -2.9626 2.9626          .25773             .25773
2        .75    -2.3590 2.3590          .42720             .68493
3       1.00    -2.0140 2.0140          .21488             .89981
```

Note that the last entry in the "cum alpha" column contains the desired power. The drift parameter must be entered using trial-and-error until the desired power is achieved. So, the final run gives a power of 0.89981.

12.30 Designing a Trial with Sequential Monitoring

The power of a sequential test depends on the timing and frequency of the interim analyzes. We now describe how these quantities are related given the following:

1. The α spending rate $\alpha = \alpha(1)$.

2. The number of interim analyzes.

3. The timing (i.e. $\tau(t_1), \tau(t_2), ..., \tau(t_p)$).

4. The desired power.

Then the drift parameter θ is completely determined. We later show that the power is an increasing function of θ.

Relation Between Sample Size and the Drift Parameter

Recall from Brownian motion that $B[\tau(t)] = \sqrt{\tau(t)}z(t)$. In general, $E[z(t)] = \sqrt{I(t)}\delta$. $z = \frac{\widehat{\delta}(t)-\delta}{\sqrt{Var(\widehat{\delta}(t))}}$, $\widehat{\delta}(t) = \bar{x}_1(t) - \bar{x}_2(t)$. $\delta = \mu_1 - \mu_2$,

$$Var[\widehat{\delta}(t)] = \frac{\sigma_1^2}{n_1(t)} + \frac{\sigma_2^2}{n_2(t)} = \sigma^2\left[\frac{1}{n_1(t)} + \frac{1}{n_2(t)}\right]$$

with a common variance.

$$I(t) = \frac{1}{Var[\widehat{\delta}(t)]} \Rightarrow z(t) = \sqrt{I(t)}\widehat{\delta}(t) \Rightarrow E[z(t)] = \sqrt{I(t)}E[\widehat{\delta}(t)] = \sqrt{I(t)}\delta.$$

$E[B[\tau(t)]] = \theta\tau(t)$. So, $\theta\tau(t) = \sqrt{\tau(t)}\sqrt{I(t)}\delta$

$$\theta = \frac{\sqrt{I(t)}\delta}{\sqrt{\tau(t)}} = \frac{\sqrt{I(t)}\delta}{\sqrt{\frac{I(t)}{I}}} = \theta = \sqrt{I}\delta.$$

Assuming equal allocation of subjects to the two groups (see page 10 of the handout), then,

$$\theta = \sqrt{I}\delta = \sqrt{\frac{n}{4\sigma^2}}\delta,$$

$$\frac{\theta}{\delta} = \sqrt{\frac{n}{4\sigma^2}} \Rightarrow n = \frac{4\theta^2\sigma^2}{\delta^2}.$$

This is done for each I.

12.31 Homework and Answers

Complete by next Monday.

1. Let x and y be any random variables and a and b be any constants. Show each of the following is true.

   (a) $Cov(ax, by) = abCov(x, y)$. Solution: $Cov(ax, by) = E(abxy) - E(ax)E(by) = ab[E(xy) - E(x)E(y)] = abCov(x, y)$.

   (b) $Cov(x, x+y) = Var(x) + Cov(x, y)$. Solution: $Cov(x, x+y) = E[x(x+y)] - E(x)E(x+y) = E(x^2 + xy) - E(x)[E(x) + E(y)] = E(x^2) + E(xy) - [E(x)]^2 - E(x)E(y) = Var(x) + Cov(x, y)$.

2. Let $S_i = \sqrt{\tau(t_i)}$. $Z(t_i), i = 1, 2, ..., p$ where $\tau(t_i)$ are constants with $0 \le \tau(t_1) < \tau(t_2) < \cdots < \tau(t_p) \le 1$. Assume that $X_i = S_i - S_{i-1}, i = 1, 2, ..., p$ are independent random variables with means and variances $E(X_i) = 0, i = 1, 2, ..., p$ and $Var(X_i) = \tau(t_i) - \tau(t_{i-1}), i = 1, 2, ..., p$. In particular, $E(X_1) = 0, Var(X_1) = \tau(t_1)$. Show that $Cov[z(t_1), z(t_2)] = \sqrt{\frac{\tau(t_1)}{\tau(t_2)}}$. Hint, use the results in Exercise

1. Solution:

$$Cov(z(t_1), z(t_2)) = Cov\left[\frac{1}{\sqrt{\tau(t_1)}}S_1, \frac{1}{\sqrt{\tau(t_2)}}S_2\right] = \frac{1}{\sqrt{\tau(t_1)\tau(t_2)}}Cov(x_1, x_1 + x_2) =$$

$$Var(x_1) + Cov(x_1, x_2) = Var(x_1)$$

because x_1 and x_2 are independent. Thus,

$$Cov(z(t_1), z(t_2)) = \frac{1}{\sqrt{\tau(t_1)\tau(t_2)}}Var(x_1) = \frac{\tau(t_1)}{\sqrt{\tau(t_1)\tau(t_2)}} = \sqrt{\frac{\tau(t_1)}{\tau(t_2)}}$$

3. Consider a one sample clinical study to evaluate a new treatment. The standard treatment has success probability 0.50. The study is conducted to test $H_0 : \Pi = 0.50$, versus $H_1 : \Pi > 0.50$. Let n denote the total number of subjects that are planned to enter the study. For the i-th subject, let $x_i = 1$ if the treatment is a success and $x_i = -1$ otherwise. Then, $x_1, x_2, ...$ are iid random variables with the following discrete distribution.

x	-1	1
$f(x)$	$1-\Pi$	Π

Let the total planned sample size be $n = 1,000$. The entry of subjects is staggered over a 2 year period with the trial terminating after 3 years. Let $n(t)$ denote the number of responses observed by calendar time t. Let $\widehat{\delta}(t) = \sum_{i=1}^{n(t)} x_i/n(t)$. Determine

(a) $E(\widehat{\delta}(t))$. Solution: $E(x) = 1(\pi)+(-1)(1-\pi) = 2\pi-1$. $Var(x) = E(x^2)-[E(x)]^2 = 1-(2\pi-1)^2 = 4\pi(1-\pi)$ since $E(x^2) = \pi + 1 - \pi = 1$. So, $E[\widehat{\delta}(t)] = E(x) = 2\pi - 1$.

(b) $Var_{H_0}(\widehat{\delta}(t))$. Solution: $Var_{H_0}(\widehat{\delta}(t)) = \frac{Var_{H_0}(\widehat{\delta}(x))}{n(t)} = \frac{4(\frac{1}{2})(\frac{1}{2})}{n(t)} = \frac{1}{n(t)}$.

(c) $I_0(t) = [Var_{H_0}(\widehat{\delta}(t))]^{-1}$. Solution: $I_0(t) = n(t)$.

(d) $\tau(t) = \frac{I_0(t)}{I}$ where I is the information obtained when the responses of all $n = 1,000$ subjects are observed. Solution:
$I = I_0(t_p) = n$, $\tau(t) = \frac{I_0(t)}{I} = \frac{n(t)}{n}$.

4. Let group 1 be the subjects that are given a new treatment, and group 2 be the subjects that are given a standard treatment. Each subjects' response (success or failure) can only be observed 6 months after the initiation of treatment, which begins the moment a subject is randomized. The parameters: p_i is the success probability for subjects in group i. $n_i(t)$ is the number of observations accumulated on subjects in group i by time t. $n = n_1 + n_2$ where n_i is the total number of observations accumulated on subjects in group i when the trial terminates. Assumptions:

(a) Approximately equal allocation is maintained during the course of the trial (i.e. $n_1(t) = n_2(t)$ for all t).

(b) Subjects are randomized every 6 months in groups of equal size m until the end of a 2 year period. Thus, $n = 5m$, and the trial duration is 2.5 years.

(c) The standard treatment is known to have success probability $p_2 = 0.20$. It is anticipated that the new treatment will have a success rate $p_1 = 0.30$.

(a) Determine the boundaries needed to monitor the trial results at 6, 12, 18, 24 and 30 months after the trial starting date. The boundaries are to be determined for a one-sided test of $H_0 : \delta = 0$, versus $H_1 : \delta > 0$ with $\alpha = 0.05$, $\delta = p_1 - p_2$, and when using the O'Brien Flemming spending rate function. The last group of subjects is randomized at 24 months but their response to treatment can not be observed until 30 months after the trial begins. You must first determine $\tau(t)$ at $t = 6, 12, ...$ under assumptions (1) and (2) from the formula

$$\tau(t) = \frac{\frac{1}{n_1} + \frac{1}{n_2}}{\frac{1}{n_1(t)} + \frac{1}{n_2(t)}}.$$

Solution:

$$\tau(t) = \frac{\frac{1}{n_1} + \frac{1}{n_2}}{\frac{1}{n_1(t)} + \frac{1}{n_2(t)}}.$$

So, if equal allocation is maintained approximately at all times, then, $n_1 = n_2, n_1(t) = n_2(t), \tau(t) = \frac{\frac{2}{n_1}}{\frac{2}{n_1(t)}} \Rightarrow \tau(t) = \frac{n_1(t)}{n_1} = \frac{n_1(t)+n_2(t)}{n_1+n_2}$, $n = n_1 + n_2 = 5M, \tau(t_i) = \frac{iM}{5M}, i = 1, 2, 3, 4, 5$.

Calendar Time	$\tau(t_i)$	Boundaries
6	$\frac{M}{5M} = 0.20$	4.23
12	$\frac{2M}{5M} = 0.40$	2.89
18	$\frac{3M}{5M} = 0.60$	2.30
24	$\frac{4M}{5M} = 0.80$	1.96
30	$\frac{5M}{5M} = 1.00$	1.74

(b) Use the boundaries obtained in Part (a) and the program disk to determine the value of the drift parameter so the test in Part (a) has a power of 0.90. Determine the value of θ accurate to the nearest hundredth of a unit. Solution:

θ	Power
3.00	0.90448
2.97	0.89933
2.98	0.90107

So, choose $\theta = 2.97$ since it is closest to 0.90.

(c) What sample size n is needed so the one-tailed test in Part (a) has a power of 0.90? When $p_1 = 0.30$ and $p_2 = 0.20$? Solution: $n = \frac{4\theta^2 \bar{p}(1-\bar{p})}{\delta^2}$, where $\bar{p} = \frac{p_1+p_2}{2} = \frac{0.30+0.20}{2} = 0.25$. $\delta = p_1 - p_2 = 0.30 - 0.20 = 0.10$. Then, $n = \frac{4(2.97)^2(0.25)(0.75)}{(0.10)^2} = 661.57$

12.32 Final Exam Review

Our final exam is scheduled for Monday, May 5, 7-10pm, BAL 408. The exam consists of about 7 short answer questions and 3 problems on the following topics:

1. Definitions of some terms common to the area of clinical trials: double blinded trial, trial time, analysis by intent to treat, baseline measurements, withdrawals.

2. Blocked randomization: disadvantages of a block size too small and too large. Be able to explain how to use blocked randomization to allocate subjects to two treatment groups.

3. Be able to clearly distinguish between phase II and phase III trials.

4. Know the general criteria used to define the study population.

5. Which of the following variables should not be used as an explanatory variable to adjust the log rank statistic? Measurements after randomization, analysis by compliance, etc.

6. Be able to apply the analysis by intent to treat principle to a specific example to decide on an appropriate course of action.

7. Be able to apply the δ method to some statistic.

8. Be able to interpret the hazard ration $\phi = \frac{\lambda_1(x)}{\lambda_2(x)}$ for the purpose of determining the correct rejection region for a one-tailed log rank test (see Peto, et. al, 1977).

9. Sample size calculation.

10. Sequential methods: information fractions, fractions, exit probabilities, $\alpha(t_i)$.

12.33 References

1. $\beta-$Blocker Heart Attack Trial Research Group, "A Randomized Trial of Propranolol in Patients with Acute Myocardial Infarction," *Journal of the American Medical Association,* March 26, 1982, Vol 247, No. 12.

2. Gordon Lan, K. K., and Zucker, David M., "Sequential Monitoring of Clinical Trials: The Role of Information and Brownian Motion," *Statistics in Medicine,* Vol. 12, pages 753-765, 1993.

3. Peto, R., Pike, M. C., Armitage, P., et al, "Design and Analysis of Randomized Clinical Trials Requiring Prolonged Observation of Each Patient," *Br. J. Cancer,* 1977, Vol 35, No. 1.

4. Reboussin, David M., DeMets, David L., Kim, KyungMann, Gordon Lan, K. K., "Programs for Computing Group Sequential Bounds Using the Lan-Demets Method, Version 2," University of Wisconsin, Department of Biostatistics, *Technical Report # 95,* October 1995.

Chapter 13

Mathematical Statistics I

Dr. Morgan, Old Dominion University

STAT 625, Fall 1996

Text used: Hogg, Robert V. and Allen T. Craig, *Introduction to Mathematical Statistics, 5-th edition,* Prentice Hall, Upper Saddle River, NJ, 1995

13.1 Notions from Set Theory

$$A \cap B = \{x : x \in A, \text{ and } x \in B\}$$

$$\bigcap_{j=1}^{\infty} A_j = \{x : x \in A_j \forall j\}$$

$$A \cup B = \{x : x \in A \text{ and } x \in B\}$$

$$\bigcup_{j=1}^{\infty} A_j = \{x : x \in A_j \text{ for some } j\}$$

$$A - B = A \cap B^*,$$

where B^* is the complement of B.

- Distributive Property:

$$A \cap (B \cup C) = (A \cap B) \cup (A \cap C).$$

$$A \cup (B \cap C) = (A \cup B) \cap (A \cup C).$$

- DeMorgan's Laws:

$$(A \cup B)^* = A^* \cap B^*.$$

$$(A \cap B)^* = A^* \cup B^*.$$

- Cumulative Property:

$$A \cup B = B \cup A.$$

$$A \cap B = B \cap A.$$

- Associative Property:

$$A \cup (B \cup C) = (A \cup B) \cup C.$$

$$A \cap (B \cap C) = (A \cap B) \cap C.$$

13.2 Introduction to Probability

The following is an observed phenomena: there are sets of circumstances which can be repeated, but whose outcome cannot be predicted. But after long sequences of repetitions, the relative frequencies of various events seem to approach limiting values. These limits, called *expected long-run relative frequencies,* are how we interpret probability.

Example: A coin toss.

Example: Mass measurements.

The theory of statistical inference is built on a foundation of probability. Inferences are, in fact, probability statements. We begin this course with the goal of studying those fundamental statistical entities called *random variables.* So, how do we construct a theory of probability? We have experiments of the type discussed above, called *random* or *chance experiments.* These experiments produce results called *outcomes.* The collection of all possible outcomes is called the *sample space,* denoted by Ω. Subsets of Ω are called *events.*

Example: Roll a die once. $\Omega = \{1, 2, 3, 4, 5, 6, \}$. An event might be $A = \{1, 2\}$ which is a roll less than 3.

We wish to be able to assign probabilities to the various events in a consistent and coherent manner. Certainly, the following requirements must be met: If $P(C = c)$ is the probability of the set C, then

1. $P(C = c) \geq 0$.
2. If C_1 and C_2 are two events which cannot occur simultaneously, then $P(C_1 \cup C_2) = P(C_1) + P(C_2)$ which is the probability that at least one of the events occur. More generally, if $C_1, C_2, ...$ are disjoint events, then
$$P\left(\bigcup_{j=1}^{\infty}\right) = \sum_{j=1}^{\infty} P(C_j).$$
3. $P(\Omega) = 1$.

The relationship P that assigns a probability to each event which satisfies the three conditions is called *a probability set function.* It is a naive definition because we have still not said which subsets or events the probability is defined for. Let $\Im$ be a collection of subsets of Ω. $\Im$ is said to be a $\sigma-$field of subsets of Ω if

1. $\Omega \in \Im$.
2. $C \in \Im \Rightarrow C^* \in \Im$.
3. $C_1, C_2, C_3, ... \in \Im \Rightarrow \bigcup_{n=1}^{\infty} C_n \in \Im$.

Properties of $\Im$: If $C_1, C_2, ...$ are members of $\Im$, then so are

1. $\emptyset$.
2. $C_1 \cup C_2$.
3. $C_1 \cap C_2$.
4. $C_1 - C_2$.

5. $\bigcup_{j=1}^{\infty} C_j$.
6. $\bigcap_{j=1}^{\infty} C_j$.
7. $\bigcup_{j=1}^{n} C_j$.
8. $\bigcap_{j=1}^{n} C_j$.

Our more rigorous definition of probability is as follow: a *probability set function* or *probability measure* P is a function from a $\sigma-$field $\Im$ of subsets Ω to $\Re$ satisfying:

1. $P(C) \geq 0, \forall C \in \Im$.
2. $P(\Omega) = 1$.
3. If $C_1, C_2, ...$ are disjoint members of $\Im$, then

$$P\left(\bigcup_{i=1}^{\infty} C_i\right) = \sum_{i=1}^{\infty} P(C_i).$$

A *probability space* is a triple $(\Omega, \Im, P)$ where Ω is the sample space of possible outcomes of an experiment. $\Im$ is a $\sigma-$field of subsets of Ω. P is a probability set function in $\Im$. Such a triple is inherent in every discussion of probability.

Example: Suppose $\Im$ is a $\sigma-$field containing three sets A, B, and C which intersect such a way that none of the 8 possible intersections are empty. The, $\Im$ also contains all the 8 regions and all unions of the 8 regions. $|\Im| = 2^8 = 256$.

Example: Let Ω be any set. The family of all subsets of Ω is a $\sigma-$field denoted 2^{Ω}. The family consisting of just the 2 sets $\emptyset$ and Ω is a $\sigma-$field.

Example: Let $C \subset \Omega$ and suppose $C \neq \emptyset, C \neq \Omega$. Then, $\Im = \{\emptyset, C, C^*, \Omega\}$ is a $\sigma-$field.

Example: Ω is any infinite set. $\Im$ is the family of finite complements. Then, $\Im$ is not a $\sigma-$field. e.g. $\Omega = Z$. $A_i = \{5i \ni i = 1, 2, 3, ...\}$. $B = \bigcup_{i=1}^{\infty} A_i$ is infinite. B^* is also infinite. Note that $B \notin \Im$ because $\Im$ is not a $\sigma-$field.

Why consider any $\sigma-$field other than 2^{Ω} which is the collection of all subsets of Ω? The problem is that if Ω is too large, it is sometimes impossible to construct a probability set function on 2^{Ω}. In this case there will be some events(subsets) that we cannot assign a probability to. Such problems are left to higher level courses. We briefly consider $\Omega = \Re$. The two $\sigma-$fields we will be most concerned with are:

1. The family 2^{Ω} of all subsets of Ω, whenever Ω is finite and countable.
2. The smallest $\sigma-$field containing all subsets of $\Re$ of the form $(-\infty, a]$. This is called the *Borel $\sigma-$field.* Elements are called *Borel sets.*

What kind of subsets are Borel sets? Clearly $\Re = (-\infty, \infty)$ and all sets of the form $(-\infty, a)$ by definition. We also have:

1. (a, ∞) by complementation is $(-\infty, a]$.
2. $(-\infty, a) = \bigcup_{n=1}^{\infty}(-\infty, a - \frac{1}{n}]$.

3. $[a, \infty) = (-\infty, a)^*$.
4. $[a, b] = [a, \infty) \cap (-\infty, b)$.
5. $(a, b) = (a, \infty) \cap (-\infty, b)$.
6. $(a, b] = (a, \infty) \cap (-\infty, b]$.
7. $[a, b) = [a, \infty) \cap (-\infty, b)$.

Thus, all intervals are in this $\sigma-$field. So are all singletons: $\{a\} = (-\infty, a] \cap [a, \infty)$.

Example: Three tosses of a coin. $\Omega = \{HHH, TTT, HHT, HTT, HTH, THH, TTH, THT\}$. $\Im = 2^\Omega$ is the collection of all subsets of Ω. Some example events are $A =$ two tails $= \{HTT, TTH, THT\}$, and $B =$ 1-st and 3-rd toss are the same $= \{HHH, TTT, HTH, THT\}$. Here is a probability set function for this experiment:

$$P(\{c\}) = \frac{1}{8}\text{for each } c \in \Omega,\ \ P(c) = \sum_{c\in\Omega} P(\{c\}) = \frac{|c|}{8} \Rightarrow P(A) = \frac{3}{8}, P(B) = \frac{1}{2}.$$

Suppose we have the following probabilities:

$$P(\{HHH\}) = \frac{27}{64}, P(\{TTT\}) = \frac{1}{64},\ \ P(\{HHT\}) = P(\{HTH\}) = P(\{THH\}) = \frac{9}{64},$$

$$P(\{TTH\}) = P(\{THT\}) = P(\{HTT\}) = \frac{3}{64},\ \ P(\Omega) = \sum_{c\in\Omega} P(\{C\}).$$

Then,

$$P(A) = \frac{3}{64} + \frac{3}{64} + \frac{3}{64} = \frac{9}{64},\ \ P(B) = \frac{27}{64} + \frac{1}{64} + \frac{9}{64} + \frac{3}{64} = \frac{5}{8}.$$

There are many other possibilities above.

Example: Choose a number at random from the interval $[0, 1]$. $\Omega = [0, 1]$. $\Im = \text{ß(Borel set)} \cap [0, 1] = \{B \cap [0, 1] \exists : B \in \text{ß}\}$. For any $A \in \Im$, define $P(A) = \int_A dx$. Then, P as defined is a probability set function. PROOF: For any $A \in \Im$,

$$P(A) = \int_A dx \geq \int_\emptyset dx \geq 0,\ \ P(\Omega) = \int_{[0,1]} dx = 1,$$

Let $A_1, A_2, ... \in \Im$ and each A_i are disjoint. Then

$$P\left(\bigcup_{i=1}^{\infty} A_i\right) = \int_{\cup_{i=1}^{\infty} A_i} dx = \sum_{i=1}^{\infty} \int_A dx = \sum_{i=1}^{\infty} P(A_i).$$

Another choice for P could be:

$$P(A) = \int_A 2x\, dx.$$

The properties of a probability set function are as follow:

1. For each $C \in \Im$, $P(C) = 1 - P(C^*)$. PROOF: $\Omega = C \cup C^*$, and $C \cap C^* = \emptyset$. $1 = P(\Omega) = P(C \cup C^*) = P(C) + P(C^*) \Rightarrow 1 - P(C^*) = P(C)$.
2. $P(\emptyset) = 0$. PROOF: In (1), put $C = \Omega$ and $C^* = \emptyset$.

3. If $C_1, C_2 \in \Im \ni: C_1 \subseteq C_2$, then $P(C_1) \leq P(C_2)$. PROOF: $C_2 = C_1 \cup (C_1^* \cap C_2)$ and $C_1 \cap (C_1^* \cap C_2) = \emptyset$. $\Rightarrow P(C_2) = P(C_1) + P(C_1^* \cap C_2) \Rightarrow P(C_2) \geq P(C_1)$.

4. For each $C \in \Im, 0 \leq P(C) \leq 1$. PROOF: Note that $\emptyset \subseteq C \subset \Omega$. By, Theorems (2), and (3), $0 = P(\emptyset) \leq P(C)$. Also Theorem (3iii) implies $P(C) \leq P(\Omega) \leq 1$.

5. If $C_1, C_2 \in \Im$, then $P(C_1) \cup C_2) = P(C_1) + P(C_2) - P(C_1 \cap C_2)$.

Theorem 1A: Let $A_1, A_2, ...$ be a finite or countable family of events in the probability space. Then,

$$P\left(\bigcup_{j=1} A_j\right) \subseteq \sum_j P(A_j).$$

PROOF: Define $B_1 = A_1, B_2 = A_2 - A_1, B_3 = A_3 - (A_1 \cup A_2), ..., B_j = A_j - (\bigcup_{k=1}^{j-1} A_k)$. Then, (a) $B_j \subseteq A_j \Rightarrow P(B_j) \leq P(A_j) \Rightarrow \sum_j P(B_j) \leq \sum_j P(A_j)$, (b) $B_j's$ are disjoint implies $\sum_j P(B_j) = P(\bigcup_j B_j)$, (c) $\bigcup_j B_j = \bigcup_j A_j$: proof: clearly $\bigcup_j B_j \subseteq A_j$. Given $w \in \bigcup_j A_j$ then $w \in A_k$ for some k. Let j be the smallest such k. Then, $w \in A_j$ and $w \notin \bigcup_{k=1}^{j-1} A_k \Rightarrow w \in B_j \Rightarrow w \in \bigcup_j B_j \Rightarrow \bigcup_j A_j \subseteq \bigcup_j B_j$. Combining (a), (b), (c) gives

$$P\left(\bigcup_j A_j\right) = P\left(\bigcup_j B_j\right) = \sum_j P(B_j) \leq \sum_j P(A_j).$$

Definition: A sequence of sets $A_1, A_2, ...$ is said to be *non-decreasing* if $A_j \subseteq A_{j+1}, \forall j$ and *non-increasing* if $A_{j+1} \subseteq A_j, \forall j$.

Definition: $\lim_{j\to\infty} A_j = \bigcup_{j=1}^{\infty} A_j$ if the $A_j's$ are non-decreasing. $\lim_{j\to\infty} A_j = \bigcap_{j=1}^{\infty} A_j$ if the $A_j's$ are non-increasing.

Theorem 2A: If $\{A_j\}$ is a monotone sequence of events in a probability space, then

$$P\left(\lim_{j\to\infty} A_j\right) = \lim_{j\to\infty} P(A_j).$$

PROOF: Suppose the $A_j's$ are non-decreasing. Define $B_1 = A_1, B_2 = A_2 - A_1, B_j = A_j - A_{j-1}$. Then the $B_j's$ are pairwise disjoint(i.e. $B_l \cap B_m = \emptyset$ for $l \neq m$). $A_j = \bigcup_{k=1}^{j} B_k$. $\lim_{j\to\infty} A_j = \bigcup_{j=1}^{\infty} A_j = \bigcup_{j=1}^{\infty} B_j$. So,

$$P\left(\lim_{j\to\infty} A_j\right) = P\left(\lim_{j\to\infty} B_j\right) = \sum_{j=1}^{\infty} P(B_j) = \lim_{j\to\infty} \sum_{k=1}^{j} P(B_k) = \lim_{j\to\infty} P\left(\bigcup_{k=1}^{j} B_k\right) = \lim_{j\to\infty} P(A_j).$$

The proof for non-increasing can be quickly done given the above proof.

13.2.1 Finite Sample Spaces

Let $\Omega = \{c_1, c_2, ..., c_n\}$ be finite. We take $\Im = 2^{\Omega}$ to be all subsets of Ω. Let p be a real value function defined on Ω satisfying

1. $p(c_i) = 0, i = 1, 2, 3, ..., n$.

2. $\sum_{i=1}^{n} p(c_i) = 1$.

Then p produces a probability set function on $\Im$ by $P(c) = \sum_{c_i \in c} p(c_i), \forall c \in \Im$. Note:

1. $P(c) \geq 0$ is clear.
2. $P\left(\bigcup_{j=1}^{k} A_j\right) = \sum_{c_i \in \bigcup_{j=1}^{k} A_j} p(c_i) = \sum_{j=1}^{k} \sum c_i \in A_j p(c_i) = \sum_{j=1}^{k} P(A_j)$.
3. $P(c) = \sum_{c \in \Omega} p(c_i) = \sum_{i=1}^{n} p(c_i) = 1$.

So, given a finite sample space, it is sufficient to specify the probability for the individual outcomes $c_1, ..., c_n$. From this a probability set function P is easily specified. A special case of the special case is when all members of Ω are equalikely. $p(c_i) = \frac{1}{n}, i = 1, 2, ..., n$. Then from any event C: $P(C) = \sum_{c_i \in C} p(c_i) = \sum_{c_i \in C} \frac{1}{n} = \frac{|C|}{|\Omega|}$. With equalilikely outcomes , calculating probabilities is as simple as counting.

Example: Five cards are dealt from an ordinary deck of 52 cards. Count the number of aces the deal produces. What is the probability that this number is 2? $\Omega = \{$ all possible subsets of 5 cards $\} = \{$ all possible 5-card hands $\}$.

$$|\Omega| = \binom{52}{5} = 2598960.$$

Let $C = \{$ all 5 card hands containing exactly 2 aces. $\}$

$$|C| = \binom{4}{2}\binom{48}{3} = 103776, \;\; P(C) = \frac{|C|}{|\Omega|} = \frac{103776}{2598960} = 0.0399.$$

13.2.2 Interpretations of Probabilities

In the above examples, nothing dictated the choices of values of P that we made. A probability space is a probability space, regardless of its validity as a model of reality. But, to make the subject worth our effort, we need to find interpretations of the abstract notions which are such that the theorems of the abstract subject become verifiable statements about the real world. A comparison with Euclidean geometry is instructive: points and lines are undefined notions satisfying certain axioms, but they do not exist in the real world. Nevertheless, there are interpretations of the notions of “point” and “line” such that the theorems in geometry become useful real-world facts. Their status as facts, of course, is less secure in the world than it is in geometry; a theorem may be indisputably true, but ultimately it is true only about the abstractions it speaks of.

A convenient real-world interpretation for the probability of an event is provided by the following observed fact: In many situations the outcome of an experiment seems to vary even though the experiment is performed repeatedly under identical conditions. but it is found that if, after each trial, the ratio of the number of occurrences of a certain outcome to the number of performances of the experiment to date is recorded, then these “relative frequencies” of occurrence of the outcome appear to tend to a limit.

Note: The above fact is not a mathematical fact; its truth cannot be proved. For example, it may be impossible to repeat an experiment under identical conditions. Indeed, it may be this impossibility that causes the observed variability. And it is impossible to know whether a finite sequence of relative frequencies is tending to a limit. But these objections do not matter; it is the apparent truth of the observed fact that makes the interpretation possible.

With the above in mind, we agree to interpret P(A) as the expected relative frequency of occurrence of A over a long series of trials of the experiment. Thus, for example, in the coin toss example, we let A be the event “1-st toss shows H, 2-nd and 3-rd tosses agree with each other,” ie $A = \{HHH, HTT\}$, then we say $P(A) = \frac{30}{64}$. We mean that if n is very large, then we expect n repetitions of the experiment to result in event A occurring on about $\frac{30}{64}n$ times.

We do not expect exactly $\frac{30}{64}n$ occurrences of A; indeed, we may occasionally observe large deviations from this expected number. But we expect large deviations to be rare. It is because of this that one way to test the validity of the function P is to perform the experiment a large number of times and see whether the observed relative frequencies of occurrence of the outcomes are close to the probabilities we assigned. In this connection, we might say that probability theory is the subject that constructs probability spaces and deduces theorems, while statistics is the subject that tests the validity of given models by comparing observed results(data) with assertions made in accordance with the above interpretation.

Example: For a group of r randomly selected people, what is the probability that their birthdays are different?

$$\Omega = \{\text{all r-tuples of birthdays chosen from 365 days}\},\ \ |\Omega| = 365^r.$$

$$C = \{\text{all r-tuples where all members are different}\},\ \ P(C) = \frac{|C|}{|\Omega|}.$$

r	probability
2	0.9973
5	0.9729
10	0.8831
20	0.5886
22	0.5243
23	0.4927
30	0.2937
35	0.1856

Example: The digits $1, 2, ..., n$ are arranged in random order. Find the probability that $1, 2, ..., k$ occur consecutively in standard order. $\frac{(n-k+1)(n-k)!}{n!} = \frac{(n-k+1)!}{n!}$. Note that for the j-th observation, $j + k - 1 \leq n \Rightarrow j \leq n - k + 1$.

13.2.3 Conditional Probability and Independence

Let $C_1, C_2 \in \Im$ and suppose $P(C_1) > 0$.

Definition: The *conditional probability* of C_2 given C_1, denoted by $P(C_2|C_1)$, is the number $P(C_2|C_1) = \frac{P(C_1 \cap C_2)}{P(C_1)}$.

Motivation: The number is intended to represent our revised view of the probability of $C_2's$ occurrence given that we know that C_1 has occurred. In terms of long run relative frequency:

- In n trials, C_1 occurs about $nP(C_1)$ times.
- Among those trials where C_1 occurs, C_2 occurs about $nP(C_1 \cap C_2)$ times.
- So, the relative frequency of C_2 among those trials where C_1 occurs is about

$$\frac{nP(C_1 \cap C_2)}{nP(C_1)} = \frac{P(C_1 \cap C_2)}{P(C_1)}.$$

Example: Given that 3 tosses of a fair coin produce at least 1 head, what is the probability that the first toss is a tail.

$$\Omega = \{HHH, HHT, HTH, THH, TTH, THT, HTT, TTT\}.$$

$$C_1 = \{HHH, HHT, HTH, THH, TTH, THT, HTT\},\ \ C_2 = \{THH, TTH, TTT, THT\}.$$

$$C_1 \cap C_2 = \{THH, THT, TTH\},\ \ P(C_2|C_1) = \frac{P(C_1 \cap C_2)}{P(C_1)} = \frac{\frac{3}{8}}{\frac{7}{8}} = \frac{3}{7}.$$

Find the probability that the first toss is a tail, given exactly one head.

$$C_1 = \{HTT, THT, TTH\},\ \ C_1 \cap C_2 = \{THT, TTH\},\ \ P(C_2|C_1) = \frac{\frac{2}{8}}{\frac{3}{8}} = \frac{2}{3}.$$

Theorem 3A: Let P be a probability set function for $(\Omega, \Im)$ and let $C_1 \in \Im$ such that $P(C_1) > 0$. Then, $P(\cdot|C_1)$ is also a probability set function for $(\Omega, \Im)$. Proof:

1. Let $C_2 \in \Im$. $P(C_2|C_1) = \frac{P(C_1 \cap C_2)}{P(C_1)} \geq 0$.
2. Let $C_2, C_3, ... \in \Im$ be pairwise disjoint. Then,

$$P\left(\bigcup_{i=2}^{\infty} C_i | C_1\right) = \frac{P\left(\bigcup_{i=2}^{\infty} C_i \bigcap C_1\right)}{P(C_1)} = \frac{P\left(\bigcup_{i=2}^{\infty} C_i \bigcap C_1\right)}{P(C_1)} = \sum_{i=2}^{\infty} \frac{P(C_i \cap C_1)}{P(C_1)} = \sum_{i=2}^{\infty} P(C_i|C_1).$$

3. $P(\Omega|C_1) = \frac{P(\Omega \cap C_1)}{P(C_1)} = \frac{P(C_1)}{P(C_1)} = 1$.

Theorem 4a: For any events $C_1, C_2, ..., C_n$ such that $P(C_1 \cap C_2 \cap \cdots \cap C_{n-1}) > 0$, we have

$$P(C_1 \cap C_2 \cap \cdots \cap C_n) = P(C_1)P(C_2|C_1)P(C_3|C_1 \cap C_2)P(C_4|C_1 \cap C_2 \cap C_3) \cdots P(C_n|C_1 \cap C_2 \cap \cdots \cap C_{n-1}).$$

The proof is simple. This theorem is called the *multiplication rule.*

Example: The older child paradox. Pick a family at random from all families with 2 children. Assume that all 4 gender distributions FF, FM, MF, MM are equalilikely. Define the following events:

$$B = \text{ both children are girls } = \{FF\},\ \ A = \text{ at least 1 girl } = \{FF, FM, MF\}.$$

$$C = \text{ older child is a girl } = \{FM, FF\}.$$

Then,

$$P(B|A) = \frac{P(A \cap B)}{P(A)} = \frac{P(B)}{P(A)} = \frac{P(\{FF\})}{P(\{FF, FM, MF\})} = \frac{\frac{1}{4}}{\frac{3}{4}} = \frac{1}{3}.$$

And,

$$P(B|C) = \frac{P(B)}{P(\{FM, FF\})} = \frac{\frac{1}{4}}{\frac{2}{4}} = \frac{1}{2}.$$

Example: Polya urn scheme. An urn has r red balls and b blue balls. A ball is drawn and replaced along with c balls of the same color. This is repeated as often as desired. NOTE: $c = 0 \Rightarrow$ sampling with replacement and $c = -1 \Rightarrow$ sampling without replacement. Let R_j be such that j-th ball drawn is red, and B_j be such that j-th ball drawn is blue which is the same as R_j^*. Then,

$$P(R_1) = \frac{r}{r+b},\ \ P(B_1) = \frac{b}{r+b},\ \ P(R_2|R_1) = \frac{r+c}{r+b+c},\ \ P(B_2|R_1) = \frac{b}{r+b+c},$$

$$P(R_3|R_1 \cap B_2) = \frac{r+c}{r+b+2c}.$$

Then,

$$P(R_1 \cap B_2 \cap R_3) = P(R_1)P(B_2|R_1)P(R_3|R_1 \cap B_2) = \left(\frac{r}{r+b}\right)\left(\frac{b}{r+b+c}\right)\left(\frac{r+c}{r+b+2c}\right).$$

Definition: A collection of sets $C_1, C_2, ...$ is a partition of Ω if $\bigcup_{i=1}^{\infty} C_i = \Omega$ and $C_i \bigcap C_j = \emptyset$.

Theorem 5A: (Law of Total Probability) Let $C_1, C_2, ...$ be a finite or countable partition of Ω into events of positive probability. Then for any event A, $P(A) = \sum_j P(A|C_j)P(C_j)$. proof:

$$\sum_j P(A|C_j)P(C_j) = \sum_j P(A \cap C_j) = P\left(\bigcup_j A \cap C_j\right) = P(A \cap \Omega) = P(A).$$

Example: In the Polya's urn scheme, what is P(2nd ball drawn is blue)?

$$P(B_2) = P(B_2|R_1)P(R_1) + P(B_2|B_1)P(B_1) = \left(\frac{b}{r+b+c}\right)\left(\frac{r}{r+b}\right) + \left(\frac{b+2}{r+b+c}\right)\left(\frac{b}{r+b}\right) =$$

$$\frac{b}{r+b} = P(B_1).$$

The next famous result, which first appeared in the 1760's, is just a combination of Theorem 4A and Theorem 5A.

Theorem 6A: (Baye's Theorem) Let $C_1, C_2, ...$ be a finite or countable partition of Ω into events of positive probability and let A be an event of positive probability. Then for any n,

$$P(C_n|A) = \frac{P(A|C_n)P(C_n)}{\sum_j P(A|C_j)P(C_j)}.$$

Definition: Events $A, B \in \Im$ are *independent* if $P(A \cap B) = P(A)P(B)$.

Motivation: If either $P(A) = 0$ or $P(B) = 0$, then $P(A \cap B) = 0 = P(A)P(B)$. Otherwise A and B are independent implies $P(A|B) = \frac{P(A \cap B)}{P(B)} = \frac{P(A)P(B)}{P(B)} = P(A)$. So, $P(A|B) = P(B)$. Now let $C_1, C_2, ..., C_n \in \Im$. We say that $C_1, C_2, ..., C_n$ are *mutually independent* if for every subset k of $\{1, 2, ..., n\}$ $P\left(\bigcap_{j \in k} C_j\right) = \prod_{j \in k} P(C_j)$. Pairwise independence does not imply mutual independence. But, mutual independence does imply pairwise independence.

Example: Two rolls of a fair die. Define the following events: $C_1 =$ 1st roll is odd,, $C_2 =$ 2nd roll is odd,, $C_3 =$ sum is odd. Then, $P(C_1) = \frac{18}{36}$, $P(C_2) = \frac{18}{36}$, and $P(C_3) = \frac{18}{36}$. $P(C_1 \cap C_2) = P(\{11, 13, 15, 31, 33, 35, 51, 53, 55\}) = \frac{9}{36} = \frac{1}{4} = P(C_2)P(C_1)$. $P(C_1 \cap C_3) = P(\{12, 14, 16, 32, 34, 36, 52, 54, 56\}) = \frac{9}{36} = \frac{1}{4} = P(C_1)P(C_3)$. $P(C_2 \cap C_3) = P(\{21, 41, 61, 23, 43, 63, 25, 45, 65\}) = \frac{9}{36} = \frac{1}{4} = P(C_2)P(C_3)$. But, $P(C_1 \cap C_2 \cap C_3) = P(\emptyset) = 0 \neq \frac{1}{8} = P(C_1)P(C_2)P(C_3)$. Thus, no mutual independence. Furthermore, on mutual independence, $P\left(\bigcap_{i=1}^{n} C_i\right) = \prod_{i=1}^{n} P(C_i)$.

Example: Define the set $C = \{1, 2, 3, 4\}$ such that

$$P(\{1\}) = \frac{2\sqrt{2}-1}{4},\ \ P(\{2\}) = \frac{1}{4},\ \ P(\{3\}) = \frac{3-2\sqrt{2}}{4},\ \ P(\{4\}) = \frac{1}{4}.$$

Define $C_1 = \{1,3\}$, $C_2 = \{2,3\}$, $C_3 = \{3,4\}$. Then,

$$C_1 \cap C_2 \cap C_3 = \{3\}, \;\; P(C_1 \cap C_2 \cap C_3) = P(\{3\}) = \frac{3-2\sqrt{2}}{4},$$

$$P(C_1)P(C_2)P(C_3) = \left(\frac{1}{2}\right)\left(\frac{2-\sqrt{2}}{2}\right)\left(\frac{2-\sqrt{2}}{2}\right) = \frac{4-4\sqrt{2}+2}{8} = \frac{3-2\sqrt{2}}{4} = P(C_1 \cap C_2 \cap C_3).$$

But,

$$P(C_1 \cap C_2) = \frac{3-2\sqrt{2}}{4} \neq \frac{2-\sqrt{2}}{4} = P(C_1)P(C_2).$$

Theorem 7A: If $C_1, C_2, ..., C_n$ are mutually independent, the so are $C_1^*, C_2, ..., C_n$. proof: Let $\{j_2, ..., j_k\} \subset \{2, 3, ..., n\}$. Then, $C_{j_2} \cap C_{j_3} \cap \cdots \cap C_{j_k} = (C_1 \cap (C_{3_2} \cap C_{j_3} \cap \cdots \cap C_{j_k})) \cup (C_1^* \cap (C_{j_2} \cap \cdots \cap C_{j_k}))$. The two sets on the right side are disjoint, so

$$P(C_{j_2} \cap C_{j_3} \cap \cdots \cap C_{j_k}) = P(C_1 \cap C_{j_2} \cap \cdots \cap C_{j_k}) + P(C_1^* \cap C_{j_2} \cap \cdots \cap C_{j_k}) \Rightarrow$$

$$P(C_{j_2})P(C_{j_3}) \cdots P(C_{j_k}) = P(C_1)P(C_{j_2}) \cdots P(C_{j_k}) + P(C_1^* \cap C_{j_2} \cap \cdots \cap C_{j_k}) =$$

$$(1 - P(C_1))P(C_{j_2})P(C_{j_3}) \cdots P(C_{j_k}) = P(C_1^* \cap C_{j_2} \cap \cdots C_{J_k}) = P(C_1^*)P(C_{j_2})P(C_{j_3}) \cdots P(C_{j_k}).$$

Clearly, the above extends to any number of complements.

13.2.4 Discrete Random Variables

It is often the case that it is difficult or bothersome to write down probability statements in terms of subsets of Ω. For instance, with the example of tossing a coin 3 times, the probability of 2 heads is written: $P(\{HHT, HTH, THH\})$. Suppose we define a function X on Ω where $X(c) = \#$ heads in c for each $c \in \Omega$. Then, instead of the above expression, we could write the probability of 2 heads as $P(X = 2) = P(\{c : X(c) = 2\})$. X as just defined is a random variable, which is a function from the sample space to the real line $\Re$ satisfying certain properties.

Example: Let Ω be all 5 card hands from a standard deck of 52 cards. If we want to know about the number of aces found in a hand, define $X(c) = \#$ aces in $c \in \Omega$. X has possible values $\{0, 1, 2, 3, 4\}$. $P(X = 3) = P(\{c : X(c) = 3\})$.

Two primary purposes for using random variables are:

1. Convince — It is much easier to write down probability statements in terms of numbers, than in terms of the sample space.

2. Restriction of attention to events of interest — Not every event can necessarily be expressed in terms of values of a particular random variable. In the coin toss experiment, "heads on first toss" can not be expressed in terms of X = "# heads in 3 tosses." But, if we are only concerned with the total number of heads, why be bothered with the other event?

Definition: A random variable X on a sample space Ω with σ-field $\Im$ is a function assigning one real number $X(c)$ to each $c \in \Omega$ so that $\{X \leq x\} = \{c : X(c) \leq x\} \in \Im$ for every $x \in \Re$(ie the inverse under X of each Borel set of $\Re$ is in the σ-field $\Im$).

Notation: $\{X \leq x\}$ is notation for $\{c : X(c) \leq x\}$. We can also write this as $X^{-1}(-\infty, x]$. In general, $\{X \in B\}$ means $\{c : X(C) \in B\}$ which can be written as $X^{-1}(B)$. Probability statements in terms of X

correspond to subsets of Ω that our probability set function is defined for.

Theorem 8A: Let X be a random variable on sample space Ω with σ-field $\Im$ and probability set function P. Then, the set function P_x on the Borel sets of $\Re$, defined by $P_x(B) = P(X^{-1}(B))$ is a probability set function. proof:

1. For any Borel set B, $P_x(B) = P(X^{-1}(B)) \geq 0$, where P is a probability set function.
2. Let $B_1, B_2, ...$ be disjoint Borel sets. Then,

$$P_x(\cup_i B_i) = P(\{c : X(c) \in \cup_i B_i\}) = P(\cup_i \{c : X(c) \in B_i\}) = \sum_i P(\{c : X(c) \in B_i\}) =$$

$$\sum_i P(X \in B_i) = \sum P_x(B_i).$$

3. $P_x(\Re) = P(X^{-1}(\Re)) = P(\Omega) = 1$ since P is a probability set function.

We have started with the triple $(\Omega, \Im, P)$. For reasons of convince, given the above, we introduce the random variable X. this gives us a new triplet $(\Re, ß, P_x)$ via the correspondence of Theorem 8A. We can now forget about $(\Omega, \Im, P)$, and think wholly in terms of $(\Re, ß, P_x)$ hence dealing only with numbers instead of the subset of some arbitrary space. It is common to drop the x subscript and write $Pr(X = 2)$ instead of $P_x(2)$. NOTE: X does not necessarily take on all real values.

Example: $(\Omega, \Im, P)$ for any fixed $A \in \Im$, define

$$I_A(c) = \begin{cases} 1 & \text{if } c \in A. \\ 0 & \text{if } c \notin A. \end{cases}$$

This is called the *indicator* of the set A. To show that I_A is a random variable, we must prove that

$$I_A^{-1}(-\infty, x] \in \Im \forall x \in \Re,$$

$$I_A^{-1}(-\infty, x] = \{c : I_A(c) \leq x\} = \begin{cases} \emptyset, & x \leq 0. \\ A^*, & 0 \leq x < 1. \\ \Omega, & x \geq 1. \end{cases}$$

The space a of I_A is $a = \{0, 1\}$.

Example: $\Omega = \{HH, TH, HT, TT\}$, $\Im = 2^\Omega$, $X(c) = \#$ heads in c, $X(HH) = 2, X(HT) = 1, X(TH) = 1, X(TT) = 0$. Check that X is a random variable:

$$X^{-1}(-\infty, x] = \begin{cases} x < 0 \Rightarrow \emptyset \\ 0 \leq x \leq 1 \Rightarrow \{HH\} \\ 1 \leq x < 2 \Rightarrow \{HT, TH, TT\} \\ x \geq 2 \Rightarrow \Omega \end{cases}$$

$a = \{0, 1, 2\}$.

Theorem 9a: Let X be a random variable on $(\Omega, \Im, P)$. Let $g : \Re \rightarrow \Re$ such that $g^{-1}(B) \in ß$ for $B \in ß$. Then, $y = g(x)$ is also a random variable. proof: given as a homework problem.

One special class of random variables is composed of what are called *discrete random variables.* A random variable with probability set function P_x on $\Re$ is called discrete if there is a function f on $\Re$ which is non-zero only on some finite or countable set a(the space of X) and

$$P_x(A) = Pr(x \in A) = \sum_{x \in A \cap a} f(x)$$

for every Borel set A.

Note:

1. $f(x) \geq 0, \forall x$ and $f(x) = 0$ for $x \notin a$.
2. $\sum_{x \in a} f(x) = 1$.

Example: $a = \{1, 3, 5, 6\}$. $f(1) = \frac{1}{4}$, $f(3) = \frac{1}{8}$, $f(5) = \frac{1}{8}$, $f(6) = \frac{1}{2}$. $f(x) = 0$ otherwise.

$$P_x((-\infty, 3]) = Pr(x \leq 3) = \sum_{x \in (-\infty,3] \cap a} f(x) = f(1) + f(3) = \frac{3}{8}.$$

$$P_x\left([2\frac{1}{2}, 3\frac{1}{2}]\right) = Pr\left(2\frac{1}{2} \leq x \leq 3\frac{1}{2}\right) = \sum_{x \in [2\frac{1}{2}, 3\frac{1}{2}] \cap a} f(x) = f(3) = \frac{1}{8}.$$

Example:

$$f(x) = \begin{cases} \left(\frac{1}{2}\right)^x, & x = 1, 2, ... \\ 0, & \text{otherwise.} \end{cases}$$

$$P_x((-\infty, 5]) = Pr(x \leq 5) = \sum_{x \in (-\infty,5] \cap a} = f(1) + f(2) + f(3) + f(4) + f(5) = \frac{31}{32}.$$

$$Pr(\ x \text{ is odd}) = \sum_{x=1,3,5} \left(\frac{1}{2}\right)^x = \sum_{y=0}^{\infty} \left(\frac{1}{2}\right)^{2y+1} = \frac{1}{2} \sum_{y=0}^{\infty} \left(\frac{1}{4}\right)^y = \frac{2}{3}.$$

Terminology: The function $f(x)$ is called the *probability density function* of the random variable x, sometimes abbreviated pdf or called simply the *density.* Some authors call this a *probability mass function.* Note: It contains all of the probability information for x.

Fact: A necessary and sufficient condition for a real valued function $f(x)$ to be the density function for a discrete random variable is

1. $f(x) \geq 0, \forall x \in \Re$ with $f(x)$ 0 only on some countable set a.
2. $\sum_{x \in a} f(x) = 1$.

Proof: Simple(restate the definition).

The distribution function of a random variable is defined as $F(x) = P(X \leq x), -\infty < x < \infty$. More details on the general properties of this function are in the next section. For a discrete random variable, it can be written

$$F(x) = \sum_{w \in a \text{ and } w \leq x} f(w).$$

Example: 3 tosses of a fair coin. X is the number of heads.

$$f(x) = \begin{cases} \frac{1}{8}, & x = 0. \\ \frac{3}{8}, & x = 1. \\ \frac{3}{8}, & x = 2. \\ \frac{1}{8}, & x = 3. \\ 0, & \text{otherwise.} \end{cases}$$

$$F(x) = \begin{cases} 0, & x < 0. \\ \frac{1}{8}, & x \leq 0. \\ \frac{1}{2}, & x \leq 1 < 2. \\ \frac{7}{8}, & x \leq 2 < 3. \\ 1, & x \geq 3. \end{cases}$$

```
       |
1     -|               .______________>
.75   -|         ._____0
.5    -|    .____0
.25   -|
       |___0
       |_______________________________
     |      |      |      |
     1      2      3      4
```

The graph is

1. A step function with jumps at the points of positive probability.
2. F is non-decreasing.
3. F is right-continuous.

$$\lim_{x \to 1^+} x = \frac{1}{2}, \text{from the right.}$$

$$\lim_{x \to 1^-} x = \frac{1}{8}, \text{from the left.}$$

13.2.5 Continuous Random Variables

A random variable with probability set function P on $\Re$ is called *continuous* if there is a non-negative function $f(x)$ on $\Re$ such that $P(X \in A) = P(A) = \int_A f(x)\,dx,$ for every Borel set A. Note:

1. $f(x) \geq 0, \forall x \in \Re$.
2. $\int_{-\infty}^{\infty} f(x)\,dx = 1$.

Note: High level courses call this type of random variable *absolutely continuous* since the probability function P is absolutely continuous with respect to Lebseque measure.

Example:

$$f(x) = \begin{cases} e^{-x}, & x > 0. \\ 0, & x \leq 0. \end{cases}$$

$$P([3,4]) = Pr(3 \leq x < 4) = \int_3^4 e^{-x}\,dx = -e^{-x}\Big|_3^4 = -e^{-4} + e^{-3} = 0.0315.$$

$$P((-\infty, 1.5)) = \int_{-\infty}^{1.5} f(x)\,dx = \int_{-\infty}^{0} e^{-x}\,dx + \int_0^{1.5} e^{-x}\,dx = 1 - e^{-1.5} = 0.7767.$$

Terminology: As with discrete random variables, all of the probability information is contained in the function $f(x)$, which is called the *probability density function* or simply the *density.* Some authors distinguish the discrete case by calling the density the *probability mass function.*

Fact: A set of necessary and sufficient conditions for a real valued function f to be a density for a continuous random variable is

1. $f(x) \geq 0, \forall x \in \Re$.
2. $\int_{-\infty}^{\infty} f(x)\,dx = 1$.

The proof requires Aratheodory's extension theorem. As with discrete random variables, we can find the distribution function $F(x) = Pr(X \leq x)$.

Example: X is a continuous random variable with density

$$f(x) = \begin{cases} \frac{2}{x^3}, & 1 < x < \infty. \\ 0, & x \leq 1. \end{cases}$$

$$F(x) = Pr(X \leq x) = \int_{-\infty}^{x} f(w)\,dw = \begin{cases} 0, & x \leq 1. \\ 1 - \frac{1}{x^2}, & x > 1. \end{cases}$$

1. This function is continuous — not a step function.
2. This function is non-decreasing.
3. This function is continuous.

13.2.6 Properties of the Distribution Function

X is any random variable. $P(A), A \in ß$ gives the probability for X defined on the Borel sets of $\Re$. The *distribution function* of X is defined as $P(X) = Pr(X \leq x) = P((-\infty, x])$ abbreviated as d.f. For discrete X, $F(X) = \sum_{w \leq x} f(w)$. For continuous X, $F(X) = \int_{-\infty}^{x} f(w)\,dw$. These are only 2 types of all possible random variables and hence of all the possible distribution functions. In fact, distribution functions *characterize* probability set functions on the real line. The properties of distribution functions are:

1. $0 \leq F(x) \leq 1$. Proof: $F(x) = Pr(X \leq x)$ is a probability.
2. $F(x)$ is a non-decreasing function of X. Proof: Let $x_1 \leq x_2$. Then,

   $$F(x_1) - F(x_2) = Pr(X \leq x_1) - Pr(X \leq x_2) = P((-\infty, x_1]) - P((-\infty, x_2) \leq 0$$

   since $(-\infty, x_1] \subseteq (-\infty, x_2]$ by Theorem 3.

3. $F(\infty) = \lim_{x\to\infty} F(x) = 1$ and $F(-\infty) = \lim_{x\to-\infty} F(x) = 0$. Proof:

$$\lim_{x\to\infty} F(x) = \lim_{x\to\infty} P((-\infty, x]).$$

Let A_x be equal to $(-\infty, x]$. The $A_x's$ are a monotone sequence of events. So by Theorem 2a,

$$P\left(\lim_{x\to\infty}(-\infty, x]\right) = P((-\infty, \infty)) = 1.$$

The proof of $F(-\infty)$ is similar.

4. $F(x)$ is a right continuous function of x. Proof:

$$\lim_{h\downarrow 0} F(x+h) = \lim_{h\downarrow 0} P((-\infty, x+h]).$$

Let $h = \frac{1}{j}$. Then, as $j \to \infty$, $h \downarrow 0$. Let $A_j = (-\infty, x + \frac{1}{j}]$. Then,

$$\lim_{h\downarrow 0} F(x+h) = \lim_{j\to\infty} P(A_j) = P\left(\lim_{j\to\infty} A_j\right) = P\left(\bigcap_{j=1}^{\infty} A_j\right) = P((-\infty, x]) = F(x).$$

Definition: A function $g(x)$ is *right continuous* at x if $\lim_{h\downarrow 0} g(x+h) = g(x)$.

We introduce two convent notations: $F(a^+) = \lim_{h\downarrow 0} F(a+h)$, and $F(a^-) = \lim_{h\uparrow 0} F(a+h)$. Right continuity says that $F(x^+) = F(x), \forall x$. However, it is not necessarily true that $F(x^-) = F(x)$. Following are probabilities for all intervals. Let $a \le b$ with $\pm\infty$ permitted.

$$P((a, b]) = F(b) - F(a).$$

$$P((a, b)) = f(b-) - F(a).$$

$$P([a, b)) = f(b-) - F(a-).$$

$$P([a, b]) = F(b) - F(a-).$$

$$P(\{a\}) = F(a) - F(a-).$$

Important Fact: It may be shown that distribution functions are characterized by these 3 properties:

1. Non-decreasing.
2. Right continuous.
3. $F(\infty) = 1$, $F(-\infty) = 0$.

That is, a function is a cdf iff it has these 3 properties. There is a 1-to-1 correspondence between functions with these 3 properties and probability set functions on $(\Re, \text{ß})$. In general, the cdf's of discrete random variables will be step functions while those of continuous random variables will be continuous functions. In fact, the Fundamental Theorem of Calculus says if $F(x) = \int_{-\infty}^{x} f(w)\,dw$, then

1. $F(x)$ is continuous at all x.
2. $F(x)$ is differentiable at least at those x for which $f(x)$ is continuous.
3. If f is continuous at x, then $\frac{\partial F(x)}{\partial x} = f(x)$.

Different densities can produce the same cdf, but those densities can differ only at a finite or countable set of points.

Example:

$$f(x) = \begin{cases} 0, & x \le 0. \\ 4x, & 0 < x < \frac{1}{2}. \\ 0, & \frac{1}{2} \le x < 1. \\ \frac{3x^2}{14}, & 1 \le x \le 2. \\ 0, & x > 2. \end{cases}$$

$$F(x) = \int_{-\infty}^{x} f(w)\,dw = \begin{cases} 0, & x \le 0. \\ 2x^2, & 0 < x < \frac{1}{2}. \\ \frac{1}{2}, & \frac{1}{2} < x < 1. \\ \frac{1}{2} + \frac{1}{14}(x^3 - 1), & 1 \le x \le 2. \\ 1, & x > 2. \end{cases}$$

The function is non-differentiable at $\frac{1}{2}$. This F has properties of a discrete and continuous random variable. It is a cdf, however.

13.2.7 Mathematical Expectation

Let x be a random variable of discrete or continuous type with pdf $f(x)$. Let $u(x)$ be a function of x. Define

$$u^+(x) = \begin{cases} u(x), & \text{if } u(x) \ge 0. \\ 0, & \text{if } u(x) < 0. \end{cases}$$

$$u^-(x) = \begin{cases} -u(x), & \text{if } u(x) < 0. \\ 0, & \text{if } u(x) \ge 0. \end{cases}$$

Clearly, $u(x) = u^+(x) - u^-(x)$. If at least one of

$$\int_{-\infty}^{\infty} u^+(x) f(x)\,dx \text{ or, } \int_{-\infty}^{\infty} u^-(x) f(x)\,dx$$

is finite, then we define the *mathematical expectation* or *expected value* of $u(x)$ as

$$E(u(x)) = \int_{-\infty}^{\infty} u(x) f(x)\,dx = E(u^+(x)) - E(u^-(x)).$$

And,

$$\sum_x u^+(x) f(x), \ \sum_x u^-(x) f(x), \ \sum_x u(x) f(x) = E(u(x))$$

for discrete cases. Otherwise, expectation is undefined. This differs from the text, which allows the expectation to be defined only if both $E(u^+(x))$ and $E(u^-(x))$ are finite. In our definition, $\int_{-\infty}^{\infty} |u(x)| f(x)\,dx$ is sufficient but not necessary for existence of the expectation. For the test, this is necessary and sufficient. Properties of mathematical expectation:

1. $u(x) = k$, then $E(u(x)) = E(k) = k$.
2. $u(x) = kv(x)$, then $E(u(x)) = E(kv(x)) = kE(v(x))$.
3. $u(x) = k_1 v_1(x) + k_2 v_2(x)$ where $v_1(x)$ and $v_2(x)$ do not have opposite infinite expectations. Then, $E(u(x)) = k_1 E(v_1(x)) + k_2 E(v_2(x))$ or if they do, k_1 and k_2 have opposite signs, then this can be generalized to a finite linear combination of functions.

Review: $E(u(x)) = \int u^+(x)f(x)\,dx - \int u^-(x)f(x)\,dx$ provided at least one of the two integrals is finite. Otherwise, the expectation does not exist.

Definition: Let m be a positive integer. The *m-th moment* of the random variable x is $E(x^m)$ provided this expectation exists.

Definition: The *n-th central limit* of the random variable x is $E[(x-E(x))^n]$, provided the expectation exists and $E(x)$ is finite.

The first moment is called the *mean* of x and is denoted by μ. So, the m-th central moment is $E((x-\mu)^m)$.

Theorem 10a: Let x be a random variable with finite mean μ.

1. If $E(x^m)$ is finite, so are $E(x^j), j = 1,2,...,m-1$, and $E((x-\mu)^j), j = 1,2,...,m$.
2. If $E((x-\mu)^m)$ is finite, so are $E(x^j), j = 1,2,...,m$, and $E((x-\mu)^j), j = 1,2,...,m-1$.

The second central moment of x is called the *variance* of x and is denoted by σ^2. $\sigma^2 = E[(x-\mu)^2]$. Note that $E[(x-\mu)^2] = E(x^2) - 2\mu E(x) + \mu^2 = E(x^2) - \mu^2$. The square root of the variance is called the *standard deviation* and is denoted by σ. $\sigma = \sqrt{E(x^2)-\mu^2}$. It is a widely used measure of dispersion. $\int (x-\mu)^2 f(x)\,dx$. The moment generating function: Let x be a random variable and suppose there exists an interval $(-h,h)$ such that the expectation $E(e^{tx})$ is finite for all $t \in (-h,h)$. Clearly this expectation is a function of t, and we write $M(t) = E(e^{xt})$. This is called the *moment generating function* of x. If x is a discrete random variable, $M(t) = \sum_x e^{tx} f(x)$. If x is a continuous random variable, $M(t) = \int_{-\infty}^{\infty} e^{tx} f(x)\,dx$.

Example: Let

$$f(x) = \begin{cases} e^{-x}, & x > 0. \\ 0, & x \leq 0. \end{cases}$$

$$M(t) = E(e^{tx}) = \int_{-\infty}^{\infty} e^{tx} f(x)\,dx = \int_0^{\infty} e^{tx} e^{-x}\,dx = \int_0^{\infty} e^{(t-1)x}\,dx = \frac{1}{t-1} e^{(t-1)x}\Big|_0^{\infty} = -\frac{1}{t-1}, \text{for } t < 1,$$

i.e.

$$M(t) = \frac{1}{t-1}, t \in (-1,1).$$

Fact: Moment generating functions(mgf), when they exist, are unique and completely determine the distribution. So, two random variables with the same mgf have the same distribution.

Now, for the continuous case(similar for discrete cases):

$$\frac{\partial M(t)}{\partial t} = M'(t) = \frac{\partial}{\partial t}\int e^{tx} f(x)\,dx = \int_{-\infty}^{\infty} \frac{\partial}{\partial t} e^{tx} f(x)\,dx = \int_{-\infty}^{\infty} e^{tx} x f(x)\,dx \Rightarrow M'(0) = \int_{-\infty}^{\infty} x f(x)\,dx = \mu.$$

$$M''(t) = \frac{\partial^2}{\partial t^2} M(t) = \int_{-\infty}^{\infty} e^{tx} x^2 f(x)\,dx \Rightarrow M''(0) = \int_{-\infty}^{\infty} x^2 f(x)\,dx = E(x^2).$$

In general,

$$M^{(m)}(t) = \frac{\partial^m}{\partial t^m} M(t) = \int_{-\infty}^{\infty} e^{tx} x^m f(x)\,dx \Rightarrow M^{(m)}(0) = E(x^m),$$

the m-th moment. Hence, the name "moment generating" function. $M(t)$ is intimately related to the Laplace transform of the density $f(x)$. We have the following result from analysis.

Theorem 11a: If $\exists h \ni M(t)$ is finite for $t \in (-h,h)$, then

1. $M(t)$ is infinitely differentiable at zero.
2. $E(x^m)$ is finite for $m = 0, 1, 2, ...$
3. $E(x^m) = M^{(m)}(0), m = 0, 1, 2, ...$

Corollary: If x has an infinite moment, then its mgf does not exist.

Example:

$$f(x) = \begin{cases} e^{-x}, & x > 0. \\ 0, & x \leq 0. \end{cases}$$

$$M(t) = \frac{1}{1-t}, |t| < 1, \;\; M'(t) = \frac{1}{(1-t)^2}, \;\; M'(0) = 1\mu, \;\; M''(t) = \frac{2}{(1-t)^3}.$$

$$M''(0) = 2 = E(x^2) \Rightarrow \sigma^2 = 2 - (1)^2 = 1.$$

Example:

$$f(x) = \begin{cases} \frac{6}{\pi^2 x^2}, & x = 1, 2, 3, ... \\ 0, & \text{elsewhere.} \end{cases}$$

$$E(x) = \sum_{x=1}^{\infty} \frac{6x}{\pi^2 x^2} = \frac{6}{\pi^2} \sum_{x=1}^{\infty} \frac{1}{x} = \infty \Rightarrow \text{ the mgf does not exist.}$$

Using a McClaurin series expansion,

$$M(t) = \sum_{m=0}^{\infty} \frac{E(x^m)t^m}{m!}.$$

Can two different distributions have all the same moments and they are all finite? If so, mgf does not exist. If not, then the moments determine the distribution.

Housdolff Moment Theorem: (see Fellier, vol 2). If a distribution is concentrated on a bounded interval, it is determined by its moments. Now consider two densities:

$$f(x) = \begin{cases} \frac{1}{\sqrt{2\pi}x} e^{-\frac{1}{2}(\log x)^2}, & x > 0. \\ 0, & x \leq 0. \end{cases}$$

$$g(x) = \begin{cases} f(x)[1 + \sin(2\pi \log x)], & x > 0. \\ 0, & x \leq 0. \end{cases}$$

You can check that

$$\int_0^{\infty} x^m f(x) \sin(2\pi \log x)\, dx = 0$$

when $m = 0, 1, 2.... \Rightarrow$ The two distributions which are clearly different, have the same moments.
Now that we have done the mathematics of expectation, let's look deeper at the motivation. Let x be a discrete random variable with density $f(x)$ on $a = \{x_1, x_2, ..., x_n\}$. According to the long run "relative frequency" interpretation of probability, $Pr(X = x_j) = f(x_j)$ leads us to "expect" that in N trials, approximately $Nf(x_j)$ of the trials will result in x_j as the value of x. So in N trials, the average value of X should approach

$$\frac{x_1 N f(x_1) + x_2 N f(x_2) + \cdots + x_n N f(x_n)}{N} = \sum_{j=1}^{n} x_j f(x_j).$$

Similarly, if $u(x)$ is a function of x, we expect about $Nf(x_j)$ occurences of $u(x_j)$ in N trials. So the average observed value of $u(x)$ will be approximately

$$\frac{u(x_1)Nf(x_1) + u(x_2)Nf(x_2) + \cdots + u(x_n)Nf(x_n)}{N} = \sum_{j=1}^{n} u(x_j)f(x_j).$$

Example: Toss a fair coin. You win x dollars if first head appears on toss x. What is your average winnings?

$$f(x) = \begin{cases} \left(\frac{1}{2}\right)^x, & x = 1, 2, ... \\ 0, & \text{elsewhere.} \end{cases}$$

The average winnings are

$$\sum_{x=1}^{\infty} x\left(\frac{1}{2}\right)^x = 2 \text{ dollars.}$$

Example: x has the pdf

$$f(x) = \begin{cases} \frac{2}{3^j}, & x = 3^j, j = 1, 2, 3, ... \\ 0, & \text{otherwise.} \end{cases}$$

$$\sum_x f(x) = \sum_{j=1}^{\infty} \frac{2}{3^j} = 2\left(\frac{\frac{1}{3}}{1-\frac{1}{3}}\right) = 1.$$

Then,

$$\sum_x xf(x) = \sum_{j=1}^{\infty} 3^j \left(\frac{1}{3^j}\right) = \sum_{j=1}^{\infty} 1 = \infty.$$

Example:

$$f(x) = \begin{cases} \frac{1}{3^j}, & x = -3^j, j = 1, 2, 3, ... \\ \frac{1}{3^j}, & x = 3^j, j = 1, 2, 3, ... \end{cases}$$

Obviously, $\sum_x f(x) = 1$. But,

$$\sum_x xf(x) \sum_{j=1}^{\infty} -3^j\left(\frac{1}{3^j}\right) + \sum_{j=1}^{\infty} 3^j\left(\frac{1}{3^j}\right) = \sum_{j=1}^{\infty} -1 + \sum_{j=1}^{\infty} 1 = -\infty + \infty \Rightarrow \text{undefined.}$$

13.2.8 Chebyshev's Inequality

Theorem 6: Let $u(x)$ be a non-negative function of x. Let c be a positive constant. Then

$$Pr(u(x) \geq c) \leq \frac{E(u(x))}{c}.$$

Proof: We prove this for the continuous case(discrete case is similar).

$$E(u(x)) = \int_{-\infty}^{\infty} u(x)f(x)\,dx = \int_A u(x)f(x)\,dx + \int_{A^c} u(x)f(x)\,dx \text{ where } A = \{x : u(x) \geq c\}.$$

$$\Rightarrow E(u(x)) \geq \int_A u(x)f(x)\,dx \geq \int_A cf(x)\,dx = c\int_A f(x)\,dx = cPr(u(x) \geq c).$$

Theorem 7: (Chebychev's Theorem) Let x be a random variable with finite variance σ^2. Then for every $k > 0$,

$$Pr(|x - \mu| \geq k\sigma) \leq \frac{1}{k^2}.$$

Proof: In Theorem 6, let $u(x) = (x-\mu)^2$ and let $c = k^2\sigma^2$. Then, Theorem 6 says

$$Pr((x-\mu)^2 \geq k^2\sigma^2) \leq \frac{E[(x-\mu)^2]}{k^2\sigma^2},$$

$$Pr(|x-\mu| \geq k\sigma) \leq \frac{\sigma^2}{k^2\sigma^2} = \frac{1}{k^2}.$$

Note: The inequality is typically not sharp. See Example 2 on page 70 of the text book where the bound is sharp.

13.3 Multivariate Distributions

Example: Consider the distribution of two random variables. Toss a coin 3 times. Define the following events: x_1 = number of heads on the first two tosses. x_2 = number of heads on all three tosses. The vector $\underline{x} = (x_1, x_2)$.

Outcome	x_1, x_2
HHH	(2,3)
HHT	(2,2)
HTH	(1,2)
THH	(1,2)
TTH	(0,1)
THT	(1,1)
HTT	(1,1)
TTT	(0,0)

The probability distribution of (x_1, x_2) is

(x_1, x_2)	$P(x_1, x_2)$
(0,0)	$\frac{1}{8}$
(0,1)	$\frac{1}{8}$
(1,1)	$\frac{2}{8}$
(1,2)	$\frac{2}{8}$
(2,2)	$\frac{1}{8}$
(2,3)	$\frac{1}{8}$

A pair of random variables (x, y) is said to be discrete, or to have a discrete distribution if there exists a function $f(x, y)$, which is non-zero only on some countable or finite 2-dimensional set a such that, $P(A) = Pr((x, y) \in A) = \sum_{(x,y)\in A\cap a} \sum f(x, y)$ for every 2 dimensional Borel set A.

Example:

x	y	$f(x,y)$
0	2	0.1
1	4	0.2
2	6	0.3
3	8	0.4

where $f(x, y) = 0$ elsewhere. $a = \{(0, 2), (1, 4), (2, 6), (3, 8)\}$ $Pr(x < 2, y \geq 3) = 0.2 = \{(1, 4)\}$ $Pr(0 \leq x \leq 1, y \leq 6) = 0.3 = \{(0, 2), (1, 4)\}$ Note: $f(x, y)$ must have $f(x, y) \geq 0, \forall (x, y), \sum_{(x,y)\in a} f(x, y) = 1$. Take the continuous case on the previous page, if $\exists$ a function $f(x, y)$ on $\Re^2 \ni$: $Pr((x, y) \in A) = \int_A \int f(x, y)\, dx\, dy$ for every 2-dimensional Borel set A, $f(x, y)$ is called the pdf of (x, y).

Example:

$$f(x,y) = \begin{cases} 6x^2y, & 0 < x < 1, \text{ or } 0 < y < 1 \\ 0, & \text{elsewhere} \end{cases}$$

$$P\left(0 < x < \frac{3}{4}, \frac{1}{3} < y < 2\right) = \int_{\frac{1}{3}}^{2} \int_{0}^{\frac{3}{4}} f(x,y)\,dx\,dy = \int_{\frac{1}{3}}^{2} \int_{0}^{\frac{3}{4}} 6x^2y\,dx\,dy = \int_{\frac{1}{3}}^{2} y2x^3\Big|_0^{\frac{3}{4}} dy = 2x^3\Big|_0^{\frac{3}{4}} \times \frac{y}{2}\Big|_{\frac{1}{3}}^{1} = \frac{3}{8}.$$

$$Pr(x < y) = \int_{x<y}\int f(x,y)\,dx\,dy = \int_0^1 \int_0^y 6x^2y\,dx\,dy = \int_0^1 y2x^3\Big|_0^y dy = \int_0^1 2y^4\,dy = \frac{2}{5}y^5\Big|_0^1 = \frac{2}{5}.$$

Note: Borel sets of $\Re^2$ consist of those sets in the smallest σ-field containing all sets of the form $(-\infty, x_1] \times (-\infty, x_2]$, (all x_1, x_2). Equivalently, this is all products $B_1 \times B_2$ where B_1 and B_2 are Borel sets of $\Re^1$.

Example:

$$f(x,y) = \begin{cases} 2, & 0 < x < y < 1 \\ 0, & \text{elsewhere} \end{cases}$$

Is this a density?

$$\int_0^1 \int_0^y 2\,dx\,dy = \int_0^1 2x\Big|_0^y dy = \int_0^1 2y\,dy = y^2\Big|_0^1 = 1.$$

Find

$$Pr\left(x > \frac{1}{2}\right) = Pr\left(x > \frac{1}{2}, x < y < 1\right) = \int_{\frac{1}{2}}^{1} \int_{\frac{1}{2}}^{y} 2\,dx\,dy = \int_{\frac{1}{2}}^{1} 2x\Big|_{\frac{1}{2}}^{y} dy =$$

$$\int_{\frac{1}{2}}^{1} (2y-1)\,dy = y^2 - y\Big|_{\frac{1}{2}}^{1} = 1 - 1 - \frac{1}{4} + \frac{1}{2} = \frac{1}{4}.$$

13.4 Homework

13.5 More on Two Random Variables

Let (x, y) be a pair of random variables. We define their distribution function as $F(x, y) = Pr(X \leq x, Y \leq y)$. If x and y are both continuous, then $F(x, y) = \int_{-\infty}^{x}\int_{-\infty}^{y} f(v, w)\,dw\,dv$. If they are both discrete, then $F(x, y) = \sum_{V \leq x}\sum_{W \leq y} f(v, w)$.

The following can be checked:

1. $F(x, y)$ is non-decreasing in each argument.
2. $\lim_{x\to\infty, y\to\infty} F(x, y) = 1$. $\lim_{x\to-\infty} F(x, y) = 0 = \lim_{y\to-\infty} F(x, y)$.

3. $F(x,y)$ is right continuous in each argument.
4. Prove for Homework: For any $A < b$ and $C < d$, $Pr(A < x \le b, C < y \le d) = F(b,d) - F(b,C) - F(A,d) + F(A,d)$.

Example: Let

$$f(x,y) = \begin{cases} 2e^{-x-2y}, & x > 0, y > 0. \\ 0, & \text{otherwise.} \end{cases}$$

$$\int_0^X \int_0^y 2e^{-v-2w}\,dw\,dv = \int_0^x e^{-v}\left[\int_0^y 2e^{-2w}\,dw\right] dv =$$

$$\int_0^x e^{-v}\left[-e^{-2w}\right]_0^y dv = (1-e^{-2y})\int_0^x e^{-v}\,dv = (1-e^{-2y})(1-e^{-x}).$$

i.e.

$$F(x,y) = \begin{cases} (1-e^{-2y})(1-e^{-x}), & x > 0, y > 0. \\ 0, & \text{elsewhere.} \end{cases}$$

When discussing the pair of random variables (x,y), we will speak of the *joint density function* $f(x,y)$ and the *joint distribution function* $F(x,y)$. This is to distinguish them from the corresponding functions for x and y alone which will be called *marginal densities* and *distributions.* For example, the joint pdf of (x,y) is $f(x,y)$. Let's find the density for y alone:

$$Pr(Y \le y) = Pr(-\infty < x < \infty, Y \le y) = \int_{-\infty}^{y}\int_{-\infty}^{\infty} f(x,y)\,dx\,dy,$$

where $\int_{-\infty}^{\infty} f(x,y)\,dx$ is the density for y. We make two observations:

1. The marginal density for y is $f(y) = \int_{-\infty}^{\infty} f(x,y)\,dx$, and for x $f(x) = \int_{-\infty}^{\infty} f(x,y)\,dy$.
2. The marginal distribution function for y is $F(y) = \lim_{x\to\infty} F(x,y)$, and for x $F(x) = \lim_{y\to\infty} F(x,y)$.

Example:

$$f(x,y) = \begin{cases} 2e^{-x}e^{-2y}, & x > 0, y > 0. \\ 0, & \text{elsewhere.} \end{cases}$$

The marginal density of x is

$$f(x) = \begin{cases} \int_0^\infty 2e^{-x}e^{-2y}\,dy = e^{-x}, & x > 0. \\ 0, & \text{otherwise.} \end{cases}$$

The marginal cdf of x is

$$F(x) = \lim_{y\to\infty} F(x,y) = \lim_{y\to\infty}(1-e^{-x})(1-e^{-2y}) = \begin{cases} 1-e^{-x}, & x > 0. \\ 0, & \text{elsewhere.} \end{cases}$$

Example: Toss a coin 3 times. Let x_1 be the number of heads on the first 2 tosses. Let x_2 be the total number of heads. The joint distribution is as follow:

$f(x,y)$	0	1	2
0	$\frac{1}{8}$	0	0
1	$\frac{1}{8}$	$\frac{1}{4}$	0
2	0	$\frac{1}{4}$	$\frac{1}{8}$
3	0	0	$\frac{1}{8}$

$$f_1(x_1) = \sum_{x_2} f(x_1, x_2) = \begin{cases} \frac{1}{4}, & x_1 = 0. \\ \frac{1}{2}, & x_1 = 1. \\ \frac{1}{4}, & x_1 = 2. \end{cases}$$

$$f_2(x_2) = \sum_{x_1} f(x_1, x_2) = \begin{cases} \frac{1}{8}, & x_2 = 0. \\ \frac{3}{8}, & x_2 = 1. \\ \frac{3}{8}, & x_2 = 2. \\ \frac{1}{8}, & x_2 = 3. \end{cases}$$

13.6 Conditional Distributions and Expectations

Now we can define conditional probabilities for values of random variables in terms of densities. First consider x_1 and x_2 are discrete. Let A_1 and A_2 be events $A_1 = \{X_1 = x_1\} = \{X_1 = x_1, -\infty < x_2 < \infty\}$ and $A_2 = \{X_2 = x_2\} = \{X_2 = x_2, -\infty < x_1 < \infty\}$. By definition, $P(A_2|A_1) = \frac{P(A_1 \bigcap A_2)}{P(A_1)} = \frac{P(X_1 = x_1 \text{ and } X_2 = x_2)}{P(X_1 = x_1)} = \frac{f(x_1,x_2)}{f_1(x_1)}$. Hence, define the conditional density x_2 given x_1 as $\frac{f(x_1,x_2)}{f(x_1)}$, (whenever $f_1(x_1) > 0) = f(x_2|x_1)$. Likewise, the conditional density of x_1 given x_2 is $\frac{f(x_1,x_2)}{f(x_2)} = f(x_1|x_2)$, when $f_(x_2) > 0$. Suppose x_1 and x_2 are discrete. $f(x_1, x_2)$ is the joint density. The conditional density of x_2 given x_1 is $f(x_2|x_1) = \frac{f(x_1,x_2)}{f_1(x_1)}$, defined when $f_1(x_1) > 0$. The c.d. of x_1 given x_2 is $f(x_1|x_2) = \frac{f(x_1,x_2)}{f_2(x_2)}$, defined when $f_2(x_2) > 0$.. Conditional densities for discrete random variables given the probability for one random variable given that the other takes a specific value. A conditional density for discrete random variables has the properties on any discrete random variable density:

1. $f(x_2, |x_1) \geq 0, \forall x_2$ and $f(x_2|x_1) > 0$ only for x_2 in a countable set.
2. $\sum_{x_2} f(x_2|x_1) = \sum_{x_2} \frac{f(x_1,x_2)}{f_1(x_1)} = \frac{1}{f_1(x_1)} \sum_{x_2} f(x_1, x_2) = 1$.

In particular, $P(X_2 = x_2|X_1 = x_1) = P(x_2|x_1)$. We now extend the above definitions to the continuous case. Let x_1 and x_2 be continuous random variables. Define: $f(x_1|x_2) = \frac{f(x_1,x_2)}{f(x_2)}$, when $f(x_2) > 0$. as the conditional density of x_1 given $X_2 = x_2$. Also, $f(x_2|x_1) = \frac{f(x_1,x_2)}{f(x_1)}$, $f(x_1) > 0$ is defined as the conditional density of x_2 given $X_1 = x_1$. NOTE WELL: $f(x_1, x_2)$ and $F(x_2|x_1)$ are not probabilities. They are densities for continuous random variables and probabilities for the continuous case are found by integration. $Pr(a <$

$x_1 < b|X_2 = x_2) = \int_a^b f(x_1|x_2)\,dx_1$. We CAN NOT write $\frac{Pr(a<x_1<b)}{Pr(X_2=x_2)}$, because the denominator is zero. Nevertheless, we are interested in the distribution of x_1 given x_2 when x_2 takes a particular value. This information is in the conditional density $f(x_1|x_2)$. We note that the conditional densities for conditional random variables satisfy the properties of any continuous random variable density:

1. $f(x_1|x_2) \geq 0, \forall x$.
2. $\int_{-\infty}^{\infty} f(x_1|x_2)dx_1 = \int_{-\infty}^{\infty} \frac{f(x_1,x_2)}{f(x_2)}\,dx_1 = 1 = \frac{f(x_2)}{f(x_2)}$.

Once we have the density functions in discrete or continuous cases, we can also talk about expectation. The mean for the distribution with density $f(x_2|x_1)$ is called the conditional expectation of X_2 given x_1. It's value is $E(x_2|x_1) = \sum_{x_2} x_2 f(x_2|x_1)$, or $E(x_2|x_1) = \int_{-\infty}^{\infty} x_2 f(x_2|x_1)\,dx_2$ which is a function of x_1. In general, if $u(x_2)$ is any function of x_2, then the conditional of $u(x_2)$ given $X_1 = x_1$ is $E(u(x_2)|x_1) = \sum_{x_2} u(x_2)f(x_2|x_1)$ or $\int_{-\infty}^{\infty} u(x_2)f(x_2|x_1)\,dx_2$.

In particular, the conditional variance of x_2 given $X_1 = x_1$ is $Var(x_2|x_1) = E\{[x_2 - E(x_2|x_1)]^2|x_1)\} = \sum_{x_2}[x_2 - E(x_2|x_1)]^2 f(x_2|x_1)$ or $\int_{-\infty}^{\infty}[x_2 - E(x_2|x_1)]^2 f(x_2|x_1)\,dx_2$.

Example: $f(x_1,x_2) = \begin{cases} x_1 + x_2, & 0 < x_1 < 1, 0 < x_2 < 1. \\ 0, & \text{otherwise.} \end{cases}$

$$f_1(x_1) = \int_0^1 x_1 + x_2\,dx_2 = x_1x_2 + \left.\frac{x_2^2}{2}\right|_0^1 = \begin{cases} x_1 + \frac{1}{2}, & 0 < x_1 < 1. \\ 0, & \text{otherwise.} \end{cases}$$

$$f_2(x_2) = \int_0^1 f(x_1,x_2) = \begin{cases} x_2 + \frac{1}{2}, & 0 < x_2 < 1. \\ 0, & \text{otherwise.} \end{cases}$$

$$E(x_2|x_1) = \int_0^1 \frac{x_2(x_1+x_2)}{x_1+\frac{1}{2}}\,dx_2 = \frac{3x_1+2}{6x_1+3}.$$

$$E(x_2^2|x_1) = \int_0^1 \frac{x_2^2(x_1+x_2)}{x_1+\frac{1}{2}}\,dx_2 = \frac{4x_1+3}{12x_1+6}.$$

$$\Rightarrow Var(x_2|x_1) = E(x_2^2|x_1) - [E(x_2|x_1)]^2 = \frac{4x_1+3}{12x_1+6} - \left(\frac{3x_1+2}{6x_1+3}\right)^2 = \frac{2(6x_1^2+6x_1+1)}{(12x_1+6)^2}.$$

The mean and variance of the conditional distribution are functions of the variable conditioned on. Hence, they may well be treated as random variables.

Theorem 1A:

a) $E(x_2) = E[E(x_2|x_1)]$. Proof:

$$E[E(x_2|x_1)] = E(u(x_1)) = \int u(x_1)f_1(x_1)\,dx_1 =$$

$$\int f_1(x_1)\int x_2x_2f(x_2|x_1)\,dx_2\,dx_1 = \int f_1(x_1)\int \frac{x_2f(x_1,x_2)}{f_1(x_1)}\,dx_2\,dx_1 =$$

$$\int\int x_2f(x_1,x_2)\,dx_2\,dx_1 = \int x_2\int f(x_1,x_2)\,dx_1\,dx_2 = \int x_2f(x_2)\,dx_2 = E(x_2).$$

b) $Var(x_2) = E[Var(x_2|x_1)] + Var[(E(x_2|x_1)]$. Proof:

$$Var(x_2|x_1) = E(x_2^2|x_1) - [E(x_2|x_1)]^2. \Rightarrow E\{E(x_2^2|x_1) - E[E(x_2|x_1)]^2\} = E(x_2^2) - E[E(x_2|x_1)]^2.$$

Also,

$$Var(E(x_2|x_1)) = E\{[E(x_2|x_1)]^2\} - \{E[E(x_2|x_1)]\}^2 = E[E(x_2|x_1)]^2 - [E(x_2)]^2.$$

Combining the two expressions,

$$\Rightarrow Var(x_2|x_1) = E(x_2^2) - [E(x_2)]^2.$$

A consequence of this is the following: Let $y = E(x_2|x_1)$. Then, y has the same mean as x_2 while the variance of y satisfies $Var(y) \leq Var(x_2)$.

Example: $x_1 =$ the number of heads on the first of two tosses. $x_2 =$ the number of heads on three tosses. The joint distribution is

		x_1		
		0	1	2
x_2	0	$\frac{1}{8}$	0	0
	1	$\frac{1}{8}$	$\frac{1}{4}$	0
	2	0	$\frac{1}{4}$	$\frac{1}{8}$
	3	0	0	$\frac{1}{8}$

The marginal distributions are:

x_1	0	1	2
$f_1(x_1)$	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{1}{4}$

and

x_2	0	1	2	3
$f_2(x_2)$	$\frac{1}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{8}$

Then,

	x_1			
$f(x_2\|x_1)$	0	1	2	
0	1	0	0	$\frac{3}{12}$
1	$\frac{1}{3}$	$\frac{2}{3}$	0	$\frac{3}{12}$
2	0	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{3}{12}$
3	0	0	1	$\frac{3}{12}$
	$\frac{4}{12}$	$\frac{4}{12}$	$\frac{4}{12}$	

$$E(x_1|x_2) = \left\{ \begin{array}{ll} 0, & x_2 = 0. \\ \frac{2}{3}, & x_2 = 1. \\ \frac{4}{3}, & x_2 = 2. \\ 2, & x_2 = 3. \end{array} \right\} = \frac{2x_2}{3}$$

and,

$$Var(x_1|x_2) = \begin{cases} 0, & x_2 = 0. \\ \frac{1}{3}(\frac{2}{3})^2 + (\frac{1}{3})^2\frac{2}{3}, & x_2 = 1. \\ \frac{2}{9}, & x_2 = 2. \\ 0, & x_2 = 3. \end{cases}$$

Then, $E(x_1) = 1$ and $E(x_2) = \frac{3}{2}$.

$$E[E(x_1|x_2)] = E\left(\frac{2x_2}{3}\right) = \frac{2}{3}E(x_2) = \frac{2}{3} \times \frac{3}{2} = 1 = E(x_1).$$

13.7 Correlation Coefficient

Let x and y be random variables with finite variances σ_1^2 and σ_2^2. Hence, they also have finite means μ_1 and μ_2. Let $u_{xy} = (x - \mu_1)(y - \mu_2)$ and consider

$$E[u(x,y)] = E[(x-\mu_1)(y-\mu_2)] = E[xy - \mu_1 y - \mu_2 x + \mu_1\mu_2] =$$
$$E(x,y) - \underbrace{\mu_1 E(y)}_{\mu_2} - \underbrace{\mu_2 E(x)}_{\mu_1} + \mu_1\mu_2 = E(x,y) - \mu_1\mu_2.$$

This is called *the covariance of* x, y, abbreviated $Cov(x,y)$. If $\sigma_1 > 0$ and $\sigma_2 > 0$, we also define the *correlation coefficient* of x, y as $Corr(x,y) = \frac{Cov(x,y)}{\sigma_1\sigma_2} = \rho$. If one of σ_1 or σ_2 is equal to zero, then we do not define the correlation.

Example:

$$f(x,y) = \begin{cases} \frac{1}{50}(x^2+y^2), & 0 < x < 2. \\ 0, & \text{elsewhere.} \end{cases}$$

Let's find $Corr(x,y)$.

$$E(x,y) = \int_1^4 \int_0^2 \frac{xy}{50}(x^2+y^2)\,dx\,dy = \frac{315}{100}.$$

$$f_1(x) = \int_1^4 \frac{x^2+y^2}{50}\,dy = \begin{cases} 3x^2 + 21, & 0 < x < 2. \\ 0, & \text{elsewhere.} \end{cases}$$

$$f_2(y) = \int_0^2 \frac{x^2+y^2}{50}\,dx = \begin{cases} \frac{\frac{8}{3}+2y^2}{50}, & 1 < y < 4. \\ 0, & \text{elsewhere.} \end{cases}$$

$$\mu_1 = E(x) = \int_0^2 \frac{x(3x^2+21)}{50}\,dx = \frac{54}{50}.$$

$$\mu_2 = E(y) = \int_1^4 \frac{y(\frac{8}{3}+2y^2)}{50}\,dy = \frac{295}{100} \Rightarrow Cov(x,y) = E(x,y) - \mu_1\mu_2 = \frac{315}{100} - \frac{54}{50} \times \frac{295}{100} = -\frac{18}{500} = -0.036.$$

$$E(x^2) = \int_0^2 \frac{x^2}{50}(3x^2+21)\,dx = \frac{188}{125} \Rightarrow Var(x) = \frac{188}{125} - \left(\frac{54}{50}\right)^2 = \frac{211}{625} = 0.3376.$$

Similarly for $y : Var(y) = 0.6015. \Rightarrow Corr(x,y) = \frac{-0.036}{\sqrt{0.3376}\sqrt{0.6015}} = -0.0799.$

Usage: ρ is commonly regarded as a measure of the intensity of the linear relationship between x and y. In the homework you will show that $-1 \leq \rho \leq 1$, if $Pr(X = a, Y = b) = 1$ for some constants a, b. Then either $\rho = 1$, or $\rho = -1$ as a is positive or negative. Hence, the limiting values of ρ are found for the pair x, y having all values on a straight line; the weaker the linear relation, the smaller $|\rho|$ will be.

Notes:

1. $Cov(x,y) = E[(x-\mu)(x-\mu)] = E[(x-\mu)^2] = Var(x). \Rightarrow Corr(x,y) = 1$
2. $Cov(ax,by) = E\{[ax - a\mu_1][by - b\mu_2]\} = abE[ax - \mu_1)(y - \mu_2)] = abCov(x,y). \Rightarrow Corr(x,y) = \frac{Cov(ax,by)}{\sqrt{Var(ax)}\sqrt{Var(by)}} = \frac{abCov(x,y)}{ab\sigma_x\sigma_y} = \frac{Cov(x,y)}{\sigma_x\sigma_y} = Corr(x,y).$

Let $x_1, ..., x_n$ be a random sample with finite variances. Then,

$$Var\left(\sum_{i=1}^n x_i\right) = E\left[\left(\sum_{i+1}^n x_i\right)^2\right] - \left[E\left(\sum x_i\right)\right]^2 =$$

$$E\left[\sum_{i=1}^n x_i^2 + \sum^n\sum_{i\neq j}^n x_i x_j\right] - \left[\sum_{i=1}^n E(x_i) + 2\sum^n\sum_{i<j}^n E(x_i)E(x_j)\right] =$$

$$\sum_{i=1}^n E(x_i^2) - \sum_{i=1}^n \left[E(x_i)\right]^2 + 2\left[\sum\sum_{i<j}^n E(x_i x_j) - \sum\sum_{i<j}^n E(x_i)E(x_j)\right] =$$

$$\sum_{i=1}^n \left[E(x_i^2) - E(x_i)^2\right] + 2\sum^n\sum_{i<j}^n \left[E(x_i, x_j) - E(x_i)E(x_j)\right] = \sum_{i=1}^n Var(x_i) + 2\sum^n\sum_{i<j}^n Cov(x_i, x_j).$$

In particular, $Var(x+y) = Var(x) + Var(y) + 2Cov(x,y)$. Now, let $y_i = a_i x_i$. Then,

$$Var\left(\sum_{i=1}^n a_i x_i\right) = Var\left(\sum_{i=1}^n y_i\right) = \sum_{i=1}^n Var(y_i) + 2\sum^n\sum_{i<j}^n Cov(y_i, y_j) =$$

$$\sum_{i=1}^n a_i^2 Var(x_i) + 2\sum^n\sum_{i<j}^n a_i a_j Cov(x_i, x_j).$$

13.8 Joint Moment Generating Functions

If $\exists h_1, h_2$ such that $E(e^{t_1 x + t_2 y})$ is finite for all $t_1 \in (-h_1, h_1)$ and for $t_2 \in (-h_2, h_2)$, then we define the joint moment generating function of x and y as $E(e^{t_1 x + t_2 y}) = M(t_1, t_2)$. Note that $M(t_1, 0) = E(e^{t_1 x}) = M(t_1)$, the mgf of x. $M(0, t_2) = E(e^{t_2 y}) = M(t_2)$ the mgf of y. Also,

$$\frac{\partial^{k+m} M(t_1, t_2)}{\partial t_1^k \partial t_2^m} = \frac{\partial^{k+m} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{t_1 x + t_2 y}}{\partial t_1^k \partial t_2^m} f(x, y)\, dx\, dy =$$

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x^k y^m e^{t_1 x + t_2 y} f(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x^k y^m f(x, y)\, dx\, dy = E(x^k y^m)$$

which is also called *a moment of order* $k + m$ for (x, y). It follows that,

$$Cov(x, y) = \frac{\partial^2}{\partial_{t_1} \partial_{t_2}} M(t_1, t_2)\bigg|_{t_1 = t_2 = 0} - \frac{\partial M(t_1, o)}{\partial_{t_1}}\bigg|_{t_1 = 0} \times \frac{\partial}{\partial t_2} M(0, t_2)\bigg|_{t_2 = 0}.$$

13.9 Independent Random Variables

We now extend our notation of independent events (section 1.4 of the text book), to independent random variables. We will do this in terms of *distribution functions* since they exist for all random variables, not just discrete or continuous.

Definition: Let the random variables x_1 and x_2 have distribution functions $F_1(x_1)$ and $F_2(x_2)$, and a joint cdf $F(x_1, x_2)$. We say that x_1 and x_2 are *independent* iff $F(x_1, x_2) = F_1(x_1) F_2(x_2), \forall x_1, x_2$. This says that $Pr(X_1 \leq x_1, X_2 \leq x_2) = Pr(X_1 \leq x_1) Pr(X_2 \leq x_2)$. Recalling that Borel sets are just countable unions, intersections, and compliments of intervals of these forms $(-\infty, x]$, it follows that x_1, x_2 are independent iff $Pr(X_1 \in A_1, X_2 \in A_2) = Pr(X_1 \in A_1) Pr(X_2 \in A_2)$ for any Borel sets A_1 and A_2. This implies that $Pr(X_1 \in A_1 | X_2 \in A_2) = Pr(X_1 \in A_1)$, and $Pr(X_2 \in A_2 | X_1 \in A_1) = Pr(X_2 \in A_2)$. So, the probability for events concerning one variable are not affected by knowledge of the other variable. Now, suppose x_1, x_2 are continuous (replace $\int$ *by* $\sum$) or discrete with densities $f_1(x_1)$ and $f_2(x_2)$. Now if continuous x_1, x_2 are independent iff

$$\int_{-\infty}^{x_1} \int_{-\infty}^{x_2} f(x_1, x_2)\, dx_1\, dx_2 = F(x_1, x_2) = F_1(x_1) F_2(x_2) = \int_{-\infty}^{x_1} f_1(x_1)\, dx_1 \int_{-\infty}^{x_2} f_2(x_2)\, dx_2 =$$

$$\int_{-\infty}^{x_2} \int_{-\infty}^{x_1} f_1(u_1) f_2(x_2)\, du_1\, du_2, \forall x_1, x_2$$

$\Rightarrow f(x_1, x_2) = f_1(x_1) f_2(x_2)$ is the joint density of (x_1, x_2). Moreover since $f_1(x_1 | x_2) = \frac{f(x_1, x_2)}{f_2(x_2)}$ it follows that independence implies (and is implied by) $f(x_1 | x_2) = f_1(x_1)$, and $f_2(x_2 | x_1) = f_2(x_2)$ i.e the conditional and marginal densities are the same.

13.10 Homework Answers

8.6) (Note: There's something wrong with the first part of the proof). Prove that:

$$E(|x - b|) = E(|x - m|) + 2 \int_m^b (b - m) f(x)\, dx.$$

proof:

$$E(|x-b|) = \int_{-\infty}^{\infty} |x-b| f(x)\,dx = \int_{-\infty}^{m} |x-b| f(x)\,dx + \int_{m}^{b} |x-b| f(x)\,dx + \int_{b}^{\infty} |x-b| f(x)\,dx.$$

$$\int_{-\infty}^{m} |x-b| f(x)\,dx + \int_{b}^{\infty} |x-b| f(x)\,dx = \int_{-\infty}^{m} (b-x) f(x)\,dx + \int_{b}^{\infty} (x-b) f(x)\,dx + \int_{m}^{b} (b-x) f(x)\,dx =$$

$$\int_{-\infty}^{m} (b-x) f(x)\,dx + \int_{b}^{\infty} (x-b) f(x)\,dx - \int_{m}^{b} (b-x) f(x)\,dx + 2\int_{m}^{b} (b-x) f(x)\,dx.$$

$$\int_{-\infty}^{m} (b-m) + (m-x) f(x)\,dx + \int_{m}^{\infty} (x-m)(m-b) f(x)\,dx =$$

$$\int_{-\infty}^{m} (m-x) f(x)\,dx + \int_{m}^{\infty} (x-m) f(x)\,dx + \int_{-\infty}^{m} (b-m) f(x)\,dx + \int_{m}^{\infty} (m-b) f(x)\,dx =$$

$$\overbrace{\int_{-\infty}^{m} |x-m| f(x)\,dx + \int_{m}^{\infty} |x-m| f(x)\,dx}^{\int_{-\infty}^{\infty} |x-m| f(x)\,dx} + \overbrace{(b-m)F(m) + (m-b)(1-F(m))}^{0 \text{ since } F(m)=\frac{1}{2}}$$

$$\Rightarrow E(|x-m|) + 2\int_{m}^{b} (b-x) f(x)\,dx.$$

1a) Prove that: $E(|x|^s) = E(|x|^r) + 1, 0 \le s \le r$.

Proof: $E(|x|^s) = \int |x|^s f(x)\,dx$.

$$\int_{-1}^{1} |x|^s f(x)\,dx + \int_{x\in[-1,1]} |x|^s f(x)\,dx \le \int_{-1}^{1} f(x)\,dx + \int_{x\notin[-1,1]} |x|^r f(x)\,dx \le$$

$$\int_{-\infty}^{\infty} f(x)\,dx + \int_{-\infty}^{\infty} |x|^r f(x)\,dx = 1 + E(|x|^r).$$

1b) Prove that: $E(|x|^m) < \infty \Leftrightarrow E(x^m) < \infty$. Obvious if m is even. If m is odd,

$$E(x^m) = -\int_{-\infty}^{0} -x^m f(x)\,dx + \int_{0}^{\infty} x^m f(x)\,dx = E(u^+(x)) - E(u(x)),$$

$$E(|x|^m) = \int_{-\infty}^{0} -x^m f(x)\,dx + \int_{0}^{\infty} x^m f(x)\,dx = E(u^+(x)) + E(u^-(x)).$$

The result is that $E(x^m)$ is finite.

1c) Given $E(x^m)$ is finite, then:

i $E(x^j) < \infty$ for $j = 1, 2, ..., m-1$. $E(x^m)$ being finite implies $E|x|^m$ is finite. Then, $E|x|^j, j < m$. Then, $E|x|^j$ is finite for $j = 1, 2, ...m-1$.

ii $E(x-\mu)^j < \infty, j = 1, 2, ..., m$.

$$E(x-\mu)^j = E\left[\sum_{k=0}^{j}\begin{pmatrix} j \\ k \end{pmatrix} x^{k-\mu+j-k}\right] = \sum_{k=0}^{j}\overbrace{\begin{pmatrix} j \\ k \end{pmatrix}}^{<\infty}\overbrace{(-\mu)^{j-k}}^{<\infty}\overbrace{E(x^k)}^{\text{finite by part (i)}}.$$

which is finite.

$E(x-b)^2$ is minimum at $b = \mu$ given $E(x)$ is finite. $E(x-b)^2 = E(x^2 - 2bx + b^2) = E(x^2) - 2bE(x) + b^2$. The $E(x^2)$ could be infinite. If $E(x^2) = \infty$, then the function is constant in b.

2.3) The Law of Total Probability: $Pr(a < x \leq b, c < y \leq d) = Pr(a < x \leq b, y \leq d) - Pr(a < x \leq b, y \leq c)$ where there is no overlap. Then, $Pr(a \leq x \leq b, y \leq d) - Pr(a < x \leq b, y \leq y \leq c)$. $Pr(x \leq b, y \leq d) - Pr(x \leq a, y \leq d) - [Pr(x \leq b, y \leq c) - Pr(x \leq a, y \leq c)] = F(b,d) - F(a,d) - F(b,c) + F(a,c)$.

13.11 Test and Answers

Work any five problems. Only the first five turned in will be graded. Turn in your copy of the test with your answers. It will be returned with your graded paper.

I. Answer the following:

(a) Define what it means for two random variables X and Y to be independent. The joint distribution function equals the product of the marginal distribution functions; i.e. $F(x,y) = F_1(x)F_2(y), \forall x, y$.

(b) List three equivalent sets of conditions for independence: two for arbitrary X and Y, and one for the special case of continuous X and Y. See notes — we made a list.

(c) Use one of your conditions in (c) to prove the following : If X and Y are continuous random variables, and u and v are functions for which the expectations exist, then,

$$E[u(X)v(Y)] = E[u(X)]E[v(Y)].$$

For continuous, independent $\Leftrightarrow f(x,y) = f_1(x)f_2(y)$. So

$$E[u(x)v(y)] = \int\int u(x)v(y)f(x,y)\,dx\,dy = E[u(x)]E(v(y)].$$

(d) Define the joint mgf $M(t_1, t_2)$ of the continuous random variables X and Y. If X and Y are independent, use (c) to prove that $M(t_1, t_2) = M(t_1, 0)M(0, t_2)$.

$$M(t_1, t_2) = E(e^{t_1x + t_2y}) \Rightarrow \begin{cases} M(t_1, 0) = E(e^{t_1x}). \\ M(0, t_2) = E(e^{t_2y}). \end{cases}$$

Then, if x and y are independent,

$$M(t_1, t_2) = E[u(x)v(y)] = E[u(x)]E(v(y)] =$$

$$M(t_1, 0)M(0, t_2).$$

II. There are 15 cards on a table, arranged in three stacks of five cards each. One stack contains three spades, one stack contains four spades, and one stack contains all spades. Each stack has been thoroughly shuffled. A stack is randomly selected and its first two cards are revealed: they are both spades.

"S" represents spades. Let c_i = i-th card turned over, and s_j = j-th stack selected.

(a) If the third card in the stack is revealed, what is the probability that it is a spade?

$$P(C_3 = S|C_1 = C_2 = S) = \frac{P(C_1 = C_2 = C_3 = S)}{P(C_1 = C_2 = S)}.$$

Find the numerator and denominator using the total law of probability.

$$P(C_1 = C_2 = C_3 = S) = \sum_{j=1}^{3} P(C_1 = C_2 = C_3 = S|S_j)P(S_j) =$$

$$\frac{\binom{3}{3}\binom{2}{0}}{\binom{5}{3}}\frac{1}{3} + \frac{\binom{4}{3}\binom{1}{0}}{\binom{5}{3}}\frac{1}{3} + \frac{\binom{5}{3}\binom{0}{0}}{\binom{5}{3}}\frac{1}{3} =$$

$$\left(\frac{1}{10} + \frac{4}{10} + \frac{10}{10}\right)\frac{1}{3} = \left(\frac{15}{10}\right)\left(\frac{1}{3}\right).$$

$$P(C_1 = C_2 = S) = \sum_{j=1}^{3} P(C_1 = C_2 = S|S_j)P(S_j) =$$

$$\frac{\binom{3}{2}\binom{2}{0}}{\binom{5}{2}}\frac{1}{3} + \frac{\binom{4}{2}\binom{1}{0}}{\binom{5}{2}}\frac{1}{3} + \frac{\binom{5}{2}\binom{0}{0}}{\binom{5}{2}}\frac{1}{3} =$$

$$\left(\frac{3}{10} + \frac{6}{10} + \frac{10}{10}\right)\frac{1}{3} = \left(\frac{19}{10}\right)\left(\frac{1}{3}\right).$$

Therefore,

$$P(C_3 = S|C_1 = C_2 = S) = \frac{\left(\frac{15}{10}\right)\frac{1}{3}}{\left(\frac{19}{10}\right)\frac{1}{3}} = \frac{15}{19}.$$

(b) What is the probability that the chosen stack is the one with the four spades? Using Baye's theorem,

$$P(S_2|C_1 = C_2 = S) = \frac{P(C_1 = C_2 = S|S_2)P(S_2)}{P(C_1 = C_2 = S)} = \frac{\left(\frac{6}{10}\right)\frac{1}{3}}{\left(\frac{19}{10}\right)\frac{1}{3}} = \frac{6}{19}.$$

III. X and Y are discrete random variables with joint density

$f(x,y)$	y: 0	1	2	$f_1(x)$
0	0	$\frac{1}{4}$	$\frac{3}{4}$	$\frac{1}{3}$
1	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{3}$
2	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{3}$
$f_2(y)$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	

(a) Give two proofs for the statement "X and Y are dependent." **Proof 1:**

$$Pr(x=0, y=0) = f(0,0) = 0.$$

$$Pr(x=0)Pr(y=0) = f_1(0)f_2(0) = \frac{1}{3}\frac{1}{3} = \frac{1}{9}.$$

$$0 \neq \frac{1}{9}.$$

Proof 2:

$$Pr(x=1|y=2) = \frac{Pr(x=1, y=2)}{Pr(y=2)} = \frac{f(1,2)}{f_2(2)} = \frac{0}{\frac{1}{3}} = 0.$$

$$Pr(x=1) = f_1(1) = \frac{1}{3}.$$

$$0 \neq \frac{1}{3}.$$

(b) Find $E(X|Y=y)$ and $Var(X|Y=y)$.

$f(x\|y)$	y: 0	1	2
0	0	$\frac{1}{4}$	$\frac{3}{4}$
1	$\frac{1}{2}$	$\frac{1}{2}$	0
2	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$

$$F(x|Y=y) = \begin{cases} E(x|y=0) = 0(0) + 1(\frac{1}{2}) + 2(\frac{1}{2}) = 1.5 \\ E(x|y=1) = 0(\frac{1}{4}) + 1(\frac{1}{2}) + 2(\frac{1}{4}) = 1.0 \\ E(x|y=2) = 0(\frac{3}{4}) + 1(0) + 2(\frac{1}{4}) = 0.5 \end{cases}$$

$$\begin{cases} E(x^2|y=0) = 0^2(0) + 1^2(\frac{1}{2}) + 2^2(\frac{1}{2}) = 2.5 \\ E(x^2|y=1) = 0^2(\frac{1}{4}) + 1^2(\frac{1}{2}) + 2^2(\frac{1}{4}) = 1.5 \\ E(x^2|y=2) = 0^2(\frac{3}{4}) + 1^2(0) + 2^2(\frac{1}{4}) = 1.0 \end{cases}$$

Therefore,

$$\begin{cases} Var(x|y=0) = 2.5 - (1.5)^2 = 0.25 \\ Var(x|y=1) = 1.5 - (1.0)^2 = 0.50 \\ Var(x|y=2) = 1.0 - (0.5)^2 = 0.75 \end{cases}$$

(c) Show by calculating both sides directly that $E[E(X|Y)] = E(X)$.

$$E\{E(x|y)\} = \sum_y E(x|Y=y)f_2(y) = 1.5\left(\frac{1}{3}\right) + 1.0\left(\frac{1}{3}\right) + 0.5\left(\frac{1}{3}\right) = 1.0.$$

$$E(x) = \sum_x x f_1(x) = 0\left(\frac{1}{3}\right) + 1\left(\frac{1}{3}\right) + 2\left(\frac{1}{3}\right) = 1.0.$$

IV. Define the *distribution function* for a random variable X. Now find the distribution function for each of the following random variables:

(a) $W =$ the result of one toss of a fair die.

$$Pr(W = w) = \begin{cases} 0 & w < 1. \\ \frac{1}{6} & 1 \leq w < 2. \\ \frac{2}{6} & 2 \leq w < 3. \\ \frac{3}{6} & 3 \leq w < 4. \\ \frac{4}{6} & 4 \leq w < 5. \\ \frac{5}{6} & 5 \leq w6. \\ 1 & w \geq 6. \end{cases}$$

(b) $Y =$ a number randomly selected from the interval $[0, 1]$.

$$Pr(Y \leq y) = \int_0^y du = \begin{cases} 0, & y \leq 0. \\ y, & 0 < y < 1. \\ 1, & y \geq 1. \end{cases}$$

(c) The function X of Y and W defined by

$$X = \begin{cases} Y & \text{if } W = 1. \\ X & \text{if } W > 1. \end{cases}$$

$$Pr(X \leq x) = Pr(X = x|w = 1)Pr(w = 1) + Pr(X \leq x|w > 1)Pr(w > 1) =$$

$$Pr(Y \leq x)\frac{1}{6} + Pr(1 < W \leq x)\frac{5}{6} = \begin{cases} 0, & x < 0. \\ \frac{x}{6}, & 0 \leq x < 1. \\ \frac{1}{6}, & 1 \leq x < 2. \\ \frac{2}{6}, & 2 \leq x < 3. \\ \frac{3}{6}, & 3 \leq x < 4. \\ \frac{4}{6}, & 4 \leq x < 5. \\ \frac{5}{6}, & 5 \leq x < 6. \\ 1, & x \geq 6. \end{cases}$$

V. P is a probability set function defined on the σ-field $\Im$ of subsets of the sample space Ω.

(a) What are the properties that define a σ-field? See notes.

(b) Use the properties listed in (a) to prove that $C_1, C_2 \in \Im \Rightarrow C_1 - C_2 \in \Im$. Proof:

$$C_1 - C_2 = C_1 \cap C_2^* = (C_1^* \cup C_2)^*,$$

$$C_1 \in \Im \Rightarrow \left.\begin{array}{c} C_1^* \in \Im. \\ C_2 \in \Im. \end{array}\right\} \Rightarrow C_1^* \cup C_2 \in \Im \Rightarrow (C_1^* \cup C_2)^* \in \Im$$

(c) What are the properties that *define* a probability set function? See notes.

(d) Use the properties listed in (c) to prove that $C_1, C_2 \in \Im\ C_1 \subseteq C_2 \Rightarrow P(C_1 - C_2) = P(C_1)P(C_2)$. **Proof:** $C_2 \subset C_1 \Rightarrow C_1 = C_2 \cup (C_1 1 \cap C_2^*)$ and $C_2 \cap (C_1 \cap C_2^*) = \emptyset \Rightarrow P(C_1) = P(C_2) + P(C_1 \cap C_2^*)$.

$$\Rightarrow P(C_1) - P(C_2) = P(\overbrace{C_1 \cap C_2^*}^{C_1 - C_2})$$

(e) Give a counterexample to prove that the property proved in (d) does not hold if the condition $C_1 \subseteq C_2$ is omitted. **Proof:** Take any experiment. Take $C_1 = \emptyset, C_2 = \Omega$. $P(C_1 - C_2) = P(\emptyset) = 0$. $P(C_1) - P(C_2) = 0 - 1 = -1$.

VI. Consider the function

$$f(x) = \begin{cases} \frac{a^{x-1}e^{-a}}{(x-1)!}, & \text{if x = 1, 2, 3, ...} \\ 0, & \text{otherwise.} \end{cases}$$

Here $a \in (0, \infty)$ is a constant.

(a) Prove that f is a density for a discrete random variable X. **Proof:** Clearly $f(x) \geq 0, \forall x$. Also,

$$\sum_{x=1}^{\infty} \frac{a^{x-1}e^{-a}}{(x-1)!} = e^{-a} \sum_{x=1}^{\infty} \frac{a^{x-1}}{(x-1)!} = e^{-a} \sum_{y=0}^{\infty} \frac{a^y e^{-a}}{y!} = e^{-a}e^a = 1.$$

(b) Find the moment generating function of X.

$$M(t) = E(e^{tx}) = \sum_{x=1}^{\infty} \frac{e^{tx}a^{x-1}e^{-a}}{(x-1)!} = e^{t-a} \sum_{x=1}^{\infty} \frac{(ae^t)^{x-1}}{(x-1)!} = e^{t-a}e^{ae^t}$$

(c) Use the moment generating function to find $E(X)$ and $var(X)$.

$$\frac{\partial}{\partial t} M(t) = M(t)[1 + ae^t]$$

Set $t = 0:$

$$M(0)(1 + a) = 1 + a = E(x).$$

$$\frac{\partial^2}{\partial t^2} M(t) = M'(t)[1 + ae^t] + M(t)ae^t.$$

Set $t = 0:$

$$(1 + a)^2 + a = E(x^2) \Rightarrow E(x^2) - [E(x)]^2 = (1 + a)^2 + a - (1 + a)^2 = a = Var(x).$$

(d) Find $E(X)$ directly.

$$F(x) = \sum_{x=1}^{\infty} \frac{xa^{x-1}e^{-a}}{(x-1)!} = a \sum_{x=2}^{\infty} \frac{a^{x-2}e^{-a}}{(x-2)!} + \sum_{x=1}^{\infty} \frac{a^{x-1}e^{-a}}{(x-1)!} = a + 1.$$

13.12 Independent RVs, Expectations, and MGFs

If x_1 and x_2 are random variables, then the following statements are equivalent notions of independence:

1. $F(x_1, x_2) = F_1(x_1)F_2(x_2), \forall x_1, x_2$.
2. $Pr(X_1 \in A_1, X_2 \in A_2) = Pr(X_1 \in A_1)Pr(X_2 \in A_2), \forall A_1, A_2$ Borel sets.
3. $Pr(X_1 \in A_1 | X_2 \in A_2) = Pr(X_1 \in A_1)$ and $Pr(X_2 \in A_2 | X_1 \in A_1) = Pr(X_2 \in A_2), \forall A_1, A_2$ Borel sets.
4. If x_1 and x_2 are either discrete or continuous, then $f(x_1, x_2) = f_1(x_1)f_2(x_2)$.
5. If x_1 and x_2 are either discrete or continuous, then $f(x_1|x_2) = f_1(x_1)$, and $f(x_2|x_1) = f_2(x_2)$.

Example:

$$f(x, y) = \begin{cases} \frac{1}{50}(x^2 + y^2), & 0 < x < 2. \\ 0, & \text{elsewhere.} \end{cases}$$

We already found that

$$f_1(x) = \begin{cases} \frac{1}{50}(3x^2 + 21), & 0 < x < 2. \\ 0, & \text{elsewhere.} \end{cases}$$

$$f_2(y) = \begin{cases} \frac{1}{50}(\frac{8}{3} + 2y^2), & 1 < y < 4. \\ 0, & \text{elsewhere.} \end{cases}$$

Then,

$$f_1(x)f_2(y) = \frac{1}{2500}(8x^2 + 42y^2 + 56 + 6x^2y^2) \neq \frac{1}{50}(x^2 + y^2) \Rightarrow x, y \text{ are dependent.}$$

Also, $f(x|y) = \frac{x^2+y^2}{\frac{8}{3}+2y^2} \neq f_1(x)$. We can make the task for determining independence of x, y even simpler in the continuous and discrete cases.

Theorem 1: Let x_1 and x_2 have a joint pdf $f(x_1, x_2)$. Then, x_1, x_2 are independent iff $f(x_1, x_2) = g(x_1)h(x_2)$ where $g(x_1) > 0$ and $h(x_2) \geq 0$. Proof: If x_1, x_2 are independent then $f(x_1, x_2) = f_1(x_1)f_2(x_2) = g(x_1)h(x_2)$. Suppose next that

$$f_1(x_1) = \int_{-\infty}^{\infty} f(x_1, x_2)\, dx_2 = \int_{-\infty}^{\infty} g(x_1)h(x_2)\, dx_2 = g(x_1) \overbrace{\int_{-\infty}^{\infty} f(x_1, x_2)\, dx_2}^{c_1} = g(x_1)c_1,$$

where c_1 is positive and $c_1 > 0$. Similarly,

$$f_2(x_2) = \int_{-\infty}^{\infty} f(x_1, x_2)\, dx_1 = \int g(x_1)h(x_2)\, dx_1 = h(x_2) \int_{-\infty}^{\infty} g(x_1)\, dx_1 = h(x_2)c_2, c_2 > 0.$$

Also,

$$1 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x_1, x_2)\, dx_1\, dx_2 = \int\int g(x_1)h(x_2)\, dx_1\, dx_2 = \overbrace{\int g(x_1)\, dx_1}^{\frac{1}{c_1}} \overbrace{\int h(x_2)\, dx_2}^{\frac{1}{c_2}}$$

$c_1c_2 = 1$. Hence $f_1(x_1)f_2(x_2) = g(x_1)c_1h(x_2)c_2 = g(x_1)h(x_2) = f(x_1,x_2)$. $\Rightarrow x_1, x_2$ are independent.

Example:

$$f(x,y) = \begin{cases} \frac{1}{5}(x^2+y^2), & 0 < x < 2, 1 < y < 4. \\ 0, & \text{elsewhere.} \end{cases}$$

The function can not be factored out as $g(x)h(y)$. Thus, x, y are not independent.

Example:

$$f(x_1,x_2) = \begin{cases} 6e^{-2x_1-3x_2}, & x_1 > 0, x_2 > 0. \\ 0, & \text{elsewhere.} \end{cases}$$

$$g(x_1) = \begin{cases} 6e^{-2x_1}, & x_1 > 0. \\ 0, & \text{elsewhere.} \end{cases}$$

$$h(x_2) = \begin{cases} 6e^{-3x_2}, & x_2 > 0. \\ 0, & \text{elsewhere.} \end{cases}$$

Then, $g(x_1) = e^{-2x_1}I_{x_1>0}$, $h(x_2) = 6e^{-3x_2}I_{x_2>0}$, Then, $f(x_1,x_2) = g(x_1)h(x_2) \Rightarrow x_1, x_2$ are independent.

Example:

$$f(x_1,x_2) = \begin{cases} 8x_1x_2, & 0 < x_1 < x_2 < 1. \\ 0, & \text{elsewhere.} \end{cases}$$

Then, $8x_1x_2I_{0<x_1<x_2<1}$ does not factor into functions of x_1, x_2 alone. Look at the range for independence.

Theorem 2: (slightly modified) If x_1, x_2 are independent, then $Pr(a < x_1 \leq b, c < x_2 \leq d) = Pr(a < x_1 \leq b)Pr(c < x_2 \leq d)$. Proof: (from the homework)

$$F(bd) - F(ad) - F(bc) + F(ac) \overbrace{=}^{indep.} F_1(b)F_2(d) - F_1(a)F_2(d) - F_1(b)F_2(c) + F_1(a)F_2(c) =$$

$$[F(_1(b) - F_1(a)][F_2(d) - F_2(c)] = Pr(a < x_1 \leq b)Pr(c < x_2 \leq d).$$

Independence can simplify expectations also.

Theorem 3: Let x_1, x_2 be independent random variables with marginals $f_1(x_1)$ and $f_2(x_2)$. Then, $E[u(x_1)v(x_2)] = E[u(x_1)]E[(v(x_2)]$. Proof: (for the continuous case. the discrete case is similar)

$$\int\int u(x_1)v(x_2)f_1(x_1)f_2(x_2)\,dx_1\,dx_2 = \left[\int u(x_1)f_1(x_1)\,dx_1\right]\left[\int v(x_2)f_2(x_2)\,dx_2\right].$$

Suppose x, y have finite variances. If they are independent, then $Cov(x,y) = E(x,y) - E(x)E(y) = E(x)E(y) - E(x)E(y) = 0$. And so,

$$Corr(x,y) = \frac{Cov(x,y)}{\sqrt{Var(x)Var(y)}} = 0.$$

Therefore, x, y are uncorrelated random variables. The converse is not true. Un-correlation does not imply independence.

Example: Let x have the pdf:

$$f(x) = \begin{cases} \frac{1}{2}, & -1 < x < 1. \\ 0, & \text{elsewhere.} \end{cases}$$

You can check that $E(x) = 0$, and $E(x^3) = 0$. Let $y = x^2$. Then, $Cov(x, y) = E(xy) - E(x)E(y) = E(x^3) - E(x)E(x^2) = 0 - 0 = 0$. Therefore, the variables are uncorrelated.

Theorem 4: Let x_1, x_2 have the joint density $f(x_1, x_2)$ with marginals $f_1(x_1)$ and $f_2(x_2)$. Also, let $M(t_1, t_2)$ be the mgf for the joint distribution. Then, x_1 and x_2 are independent iff $M(t_1, t_2) = M(t_1, 0) \times M(0, t_2)$. Proof: If x_1, x_2 are independent, then $M(t_1, t_2) = E[e^{t_1x_1+t_2x_2}] = E[e^{t_1x_1}e^{t_2x_2}] = E(e^{t_1x_11})E(x^{t_2x_2}) = M(t_1, 0)M(0, t_2)$. Part II: If $M(t_1, t_2) = M(t_1, 0) \times M(0, t_2)$, then

$$M(t_1, t_2) = M(t_1, 0)m(0, t_2) = \left[\int_{-\infty}^{\infty} e^{t_1x_1} f_1(x_1)\, dx_1\right]\left[\int_{-\infty}^{\infty} e^{t_2x_2} f_2(x_2)\, dx_2\right] =$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{t_1x_1}e^{t_2x_2} f_1(x_1)f_2(x_2)\, dx_1\, dx_2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{t_1x_1+t_2x_2} f_1(x_1)f_2(x_2)\, dx_1\, dx_2.$$

Therefore, by the uniqueness of mgf's, $f_1(x_1)f_2(x_2)$ is the joint pdf of x_1, x_2. Otherwise, $M(t_1, t_2)$ would be the mgf of some other distribution. $f(x_1, x_2) = f_1(x_1)f_2(x_2)$. Therefore, x_1, x_2 are independent.

13.12.1 Extension to Several Random Variables

Sometimes we want to consider more than two random variables for the same expression and may want to ask probability questions about the simultaneous values of several variables. Write $\underline{x}(c) = (x_1(c), x_2(c), ..., x_n(c))$ where $x_1, x_2, ..., x_n$ are each real valued functions on Ω with $\sigma-$field $\Im$.

Definition: The Borel $\sigma-$field of subsets of $\Re^n$ is the smallest $\sigma-$field containing all sets of the form

$$(-\infty, a_1] \times (-\infty, a_2] \times .... \times (-\infty, a_n] = \{(x_1, x_2, ..., x_n) \ni x_1 \leq a_1, x_2 \leq a_2, ..., x_n \leq a_n\}$$

It will be denoted by ß_n.

Definition: $\underline{x} = (x_1, ..., x_n)$ mapping Ω to $\Re^n$ is a *n-dimensional random vector* if $\underline{x}^{-1}(B) \in \Im, \forall B \in \text{ß}_n$. Here, $\underline{x}^{-1}(b) = \{c : (x_1(c), x_2(c), ..., x_n(c)) \in B\}$. It may be shown that:

Result: $\underline{x} = (x_1, x_2, ..., x_n)$ is a random vector iff each x_i is a random variable.

We define a probability set function $\underline{x}$ just as we did for a single random variable: iff B is any Borel set of $\Re^n$, i.e. $B = \{(x_1, x_2, ..., x_n) \rightarrow x_1 \in B_1, x_2 \in B_2, ..., x_n \in B_n\} = B_1 \times B_2 \times ... \times B_n$ where $B_i \in \text{ß}$, then

$$P_{\underline{x}}(B) = P(\underline{x}^{-1}(B)) = P(\{c : \underline{x}(c) \in B\}) = P(\{c : x_1(c) \in B_1, x_2(c) \in B_2, ..., x_n(c) \in B_n\}).$$

13.12.2 Discrete and Continuous Cases

The n random variables $(x_1, ..., x_n)$ are jointly discrete iff $\exists$ a function $f(x_1, x_2, ..., x_n)$ which is non-zero only on some finite or countable subset $a \in \Re^n$, such that

$$Pr((x_1, ..., x_n) \in A) = \sum ... \sum_{(x_1, x_2, ... x_n) \in A \cap a} f(x_1, ..., x_n), \forall A \in ß_n.$$

Note:

1. $f(x_1, ..., x_n) \geq 0, \forall (x_1, ..., x_n)$ only if $(x_1, ..., x_n) \in a$.

2. $\sum ... \sum_{(x_1, ... x_n) \in a} f(x_1, ..., x_n) = 1$.

(1) and (2) are necessary and sufficient for $f(x_1, ..., x_n)$ to be a pdf for a set of discrete variables.

The n random variables $x_1, x_2, ... x_n$ are said to be jointly continuous of $(x_1, ..., x_n)$ is said to be a *continuous random vector* if there exists a function $f(x_1, ..., x_n)$ on $\Re^n : Pr(x_1, ..., x_n \in A) =$

$$\int ... \int f(x_1, ..., x_n) \, dx_1 \, dx_2 ... \, dx_n$$

for every n dimensional Borel set $A \in ß^n$. Note that if f must satisfy

$$f(x_1, x_2, ..., x_n) \geq 0, \forall x_1, ..., x_n,$$

$$\int \int_{\Re^n} f(x_1, ..., x_n) \, dx_1 ... \, dx_n = 1.$$

f is called the *joint density* of $x_1, x_2, ..., x_n$.

13.12.3 Distribution Functions for n Random Variables

Given n random variables, $x_1, ..., x_n$ or the random vector $(x_1, ..., x_n)$ (think of them all at the same time not individually) be the discrete or continuous, or otherwise their *joint density function* is defined to be

$$F(x_1, ..., x_n) = Pr(X_1 \leq x_1, X_2 \leq x_2, ... X_n \leq x_n).$$

The following can be checked:

1. $F(x_1, x_2, ..., x_n)$ is non decreasing in each x_i.
2. $\lim_{x_1 \to \infty x_2 \to \infty, ... x_n \to \infty} F(x_1, x_2, ..., x_n) = 1$. $\lim_{x_i \to -\infty} F(x_1, x_2, ..., x_n) = 0$ for each x_i.
3. $F(x_1, x_2, ..., x_n)$ is right continuous in each x_i.
4. For any set $(a_1, b_1] \times (a_2, b_2] \times ... \times (a_n, b_n]$,

$$\sum \begin{pmatrix} + \\ - \end{pmatrix} F(c_1, c_2, ..., c_n)$$

is non-negative where $\sum$ is over all 2^n combinations of $c_i = a_i$ and the sign is + iff the numerator of $c_i s = a_i$ is even.

Example: $n = 1$. Then, $F(b_1) - F(a_1) = Pr(a_1 < x_1 \leq b_1)$.

Example: $n = 2$. Then,

$$F(b_1, b_2) - \overbrace{F(a_1, b_2)}^{\text{number of } a_i\text{'s is odd}} - F(b_1, a_2) + \overbrace{F(a_1, a_2)}^{\text{number of } a_i\text{'s is even}} = Pr(a_1 < x_1 \leq b_1, a_2 < x_2 \leq b_2).$$

It can be shown that (1) thru (4) are *necessary and sufficient* for a function $F(x_1, x_2, ..., x_n)$ to be a distribution function. Another important property is that letting any subset of the $x_i s$ go to ∞ produces the distribution function of the remaining xs. So, e.g., $F(\infty, \infty, x_3, ..., \infty)$ is the distribution function of x_3. $F(\infty, x_2, x_3, ..., x_n)$ is the distribution function of $(x_2, x_3, ..., x_n)$.

Example:

$$f(x, y, z) = \begin{cases} 4e^{-x-2y-2z}, & x > 0, y > 0, z > 0. \\ 0, & \text{otherwise.} \end{cases}$$

is the pdf for (x, y, z).

$$\Rightarrow F(x, y, z) = \int_0^z \int_0^y \int_0^x f(u, v, w)\, du\, dv\, dw = \begin{cases} (1 - e^{-x})(1 - e^{-2y})(1 - e^{-2z}), & x > 0, y > 0, z > 0. \\ 0, & \text{otherwise.} \end{cases}$$

$F(\infty, y, z) = (1 - e^{-2y})(1 - e^{-2z})$ is the Distribution function of (y, z). $F(\infty, \infty, z) = (1 - e^{-2z})$ is the distribution function of z.

13.12.4 Marginal Densities

$f(x_1, x_2, ..., x_n)$ is the pdf for $(x_1, x_2, ..., x_n)$. Assume continuous (discrete is similar):

$$Pr(a < x_1 < b) = Pr(a < x_1 < b, -\infty < x_2 < \infty, ..., -\infty < x_n < \infty) =$$

$$\underbrace{\int_a^b \int_{-\infty}^{\infty} .... \int_{-\infty}^{\infty} f(x_1, x_2, ..., x_n)\, dx_n\, dx_{n-1} ... dx_1}_{\textit{integrating this function of } x_1 \textit{ gives the probability for } x_1.}$$

Therefore, the marginal density of x_1 is

$$f(x_1) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} .... \int_{-\infty}^{\infty} f(x_1, x_2, ..., x_n)\, dx_2\, dx_3 ... dx_n.$$

Likewise, choose any $k < n$ of the x_i's then the joint pdf of these k variables is found by integrating over the other $n - k$ variables.

Example: $n = 6$. The joint pdf of x_2, x_4, x_5 is

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x_1, x_2, x_3, x_4, x_5, x_6)\, dx_1\, dx_3\, dx_6 = f_{2,4,5}(x_2, x_4, x_5).$$

The conditional density of x_1, x_3, x_6 given x_2, x_4, x_5 is defined as x_1, x_3, x_6 given x_2, x_3, x_5 is defined as

$$\frac{f(x_1,x_2,x_3,x_4,x_5,x_6)}{f_{2,4,5}(x_2,x_4,x_5)} = f(x_1,x_3,x_6|x_2,x_4,x_5).$$

Likewise, we can define the conditional density for $n-k$ of the x's given the other k. Conditional expectations follow naturally. e.g.

$$E(u(x_1,x_3,x_6)(x_2,x_4,x_5) = \int\int\int u(x_1,x_3,x_6)f(x_1,x_3,x_6|x_2,x_4,x_5)\,dx_1\,dx_3\,dx_6.$$

13.12.5 Joint Independence

This is the generalization of independent n variables $x_1, x_2, ..., x_n$.

Definition: Let $x_1, x_2, ..., x_n$ have marginal distributions $F_1(x_1), ..., F_n(x_n)$ and a joint distribution function $F(x_1, ..., x_n)$. These are *mutually independent* iff $F_1(x_1)F_2(x_2)...F_n(x_n) = F(x_1, x_2, ..., x_n)$. It can be shown that the following are equivalent notions of *mutual independence* of $x_1, x_2, ..., x_n$.

1. $F(x_1, x_2, ..., x_n) = F_1(x_1)F_2(x_2)\cdots F_n(x_n)$.
2. $Pr(x_1 \in A_1 \text{ and } x_2 \in A_2 \text{ and } \cdots \text{ and } x_n \in A_n) = Pr(x_1 \in A_1)Pr(x_2 \in A_2)\cdots Pr(x_n \in A_n)$.
3. If $x_{i1}, x_{i2}, ..., x_{ik}$ and $x_{j1}, x_{j2}, ..., x_{jL}$ are any partition of $x_1, x_2, ..., x_n$ then,

   $$Pr(x_{i1} \in A_{i1}, x_{i2} \in A_{i2}, ..., x_{ik} \in A_{ik}|x_{j1}\, inA_{j1}, ..., x_{jL} \in A_{jL}) = Pr(x_{i1} \in A_{i1}, x_{i2} \in A_{i2}, ..., x_{ik} \in A_{ik})$$

   for all Borel sets $A_{i1}, A_{i2}, ..., A_{iL}$.

Furthermore, if $x_1, ..., x_n$ are discrete or continuous, then

4. $(x_1, ..., x_n) = f(x_1)f(x_2)\cdots f(x_n)$.
5. $(x_{i1}, x_{i2}, ..., x_{ik}|x_{j1}, x_{j2}, ..., x_{jL}) = f(x_{i1}, x_{i2}, ..., x_{ik})$ for any partition as described in (3).

Theorems (1) - (4) can all be generalized to n mutually independent random variables. Briefly stated (see page 111 of the text book):

1. The joint density $f(x_1, x_2, ..., x_n)$ factors into the product of n non-negative functions. $f(x_1, x_2, ..., x_n) = g(x_1)h(x_2)\cdots k(x_n)$ iff mutual independence holds.
2. The probabilities for intervals multiply or are found by multiplying the marginal probabilities.
3. $E(u_1(x_1), u_2(x_2), ..., u_n(x_n)) = E(u_1(x_1))E(u_2(x_2))\cdots E(u_n(x_n))$.
4. $M(t_1, t_2, ..., t_n) = \prod_{i=1}^{n} M(0, 0, 0, t_i, 0, 0, ...)$ i.e. the joint mgf factors iff $x_1, x_2, ..., x_n$ are mutually independent.

Example: Bad luck in life: Let x_0 be your loss (pain, etc) in a particular situation. Let $x_1, ..., x_n$ be the losses of others in the same situation. Assume $x_0, x_1, ..., x_n$ are independent with the same continuous distribution. Define N to be the smallest n for which $x_{n+1} > x_0$. Now, the event $(N \geq n)$ is x_0 is the largest of $x_0, x_1, ..., x_n$. By the above assumptions,

$$Pr(N \geq n) = \frac{1}{n+1} \Rightarrow Pr(N = n) = Pr(N \geq n) - Pr(N \geq n-1) = \frac{1}{n+1} - \frac{1}{n+2} = \frac{1}{(n+1)(n+2)} \Rightarrow$$

$$E(N) = \sum_{n=0}^{\infty} n\left(\frac{1}{(n+1)(n+2)}\right) = \infty.$$

13.13 Some Homework Answers

$$P(A) = P(A_1 \cup A_3 \cup A_5) = P(A_1) + P(A_3) + P(A_5), \;\; P(A_1) = \frac{1}{6},$$

$$P(A_3) = P(\text{roll } 1 = \text{not } 6, \text{ roll } 2 < 5, \text{ roll } 3 \geq 4) = P(\text{roll } 1 = \text{not } 6)P(\text{roll } 2 < 5)P(\text{roll } 3 \geq 4) =$$

$$\frac{5}{6} \times \frac{4}{6} \times \frac{3}{6} = P(A_5) = P(\text{ roll } 1 = \text{not } 6, \text{ roll } 2 < 5, \text{ roll } 3 \geq 4, \text{ roll } 4 < 3, \text{ roll } 5 \geq 2) =$$

$$\frac{5}{6} \times \frac{4}{6} \times \frac{3}{6} \times \frac{2}{6} \times \frac{5}{6}.$$

13.14 Indicators

For any $A \subseteq \Omega$, we define the *indicator function* of A :

$$I_A(c) = \begin{cases} 1, & \text{if } c \in A. \\ 0, & \text{if } c \notin A. \end{cases}$$

We have already seen that I_A is a random variable iff $A \in \Im$. We say that A has the *Bernoulli distribution* with parameter $p = P(A)$. I_A is a discrete random variable with pdf

$$f(x) = \begin{cases} p, & x = 1. \\ 1-p, & x = 0. \\ 0, & \text{otherwise.} \end{cases}$$

$$E(I_A) = \sum_x x f(x) = 1(p) + 0(1-p) = p = P(A).$$

$$E(I_A^2) = 0^2 f(0) + 1^2 f(1) = p. \Rightarrow Var(I_A) = p - p^2 = (1-p)p.$$

Next, let events $A_1, A_2, ..., A_n$ be any n events ($A_i \in \Im$). Then,

1. $I_{A_1 \cap A_2 \cap \cdots A_n} = I_{A_1} I_{A_2} \cdots I_{A_n}$.
2. $I_{A_i}^* = 1 - I_{A_i}$.
3. $A_1, A_2, ..., A_n$ are mutually independent events iff $I_{A_1}, I_{A_2}, ..., I_{A_n}$ are mutually independent random variables.
4. $Cov(I_{A_i}, I_{A_j}) = E(I_{A_i}, I_{A_j}) - E(I_{A_i})E(I_{A_j}) = E(I_{A_i \cap A_j}) - E(I_{A_i})E(I_{A_j}) = P(A_i \cap A_j) - P(A_i)P(A_j)$.

Example: An urn contains N balls of which m are red and $N - m$ are white. n balls are drawn from the urn at random without replacement. Let x be the number of red balls in the same sample. The distribution of X is called the *hyper geometric distribution.*

$$Pr(X = x) = \begin{cases} \dfrac{\begin{pmatrix} m \\ x \end{pmatrix}\begin{pmatrix} N-m \\ n-x \end{pmatrix}}{\begin{pmatrix} N \\ n \end{pmatrix}}, & x = \max(0, m(N-m))\dots\min(n, m). \\ 0, & \text{otherwise.} \end{cases}$$

Use indicators to find the mean and variance. Let

$$I_j = \begin{cases} 1, & \text{if red ball } j \text{ is drawn.} \\ 0, & \text{otherwise.} \end{cases}$$

where the red balls in the urn are numbered $1, 2, \dots, M$. Then,

$$x = I_1 + I_2 + \cdots + I_m.$$

$$E(x) = E\left(\sum_{j=11}^{m} I_j\right) = \sum_{j=1}^{m} E(I_j) = \sum_{j=1}^{m} Pr(\text{red ball } j \text{ drawn}) = \sum_{j=1}^{m} Pr(\text{red ball 1 drawn}) =$$

$$mPr(I_1 = 1) = \frac{mn}{N}. \text{ see next page.}$$

$$Var(x) = Var\left(\sum_{j=1}^{m} I_j\right) = \sum_{j=1}^{m} Var(I_j) + 2\sum\sum_{j<j'} Cov(I_j, I_{j'}) =$$

$$\sum_{j=1}^{m} P(I_j = 1)[1 - P(I_j = 1)] + 2\sum\sum_{j<j'}[P(I_j I_{j'} = 1) - P(I_j = 1)P(I_{j'} = 1)] =$$

$$MPr(I_1 = 1)[(1 - Pr(I_1 = 1)] + 2\begin{pmatrix} m \\ 2 \end{pmatrix}\Big[Pr(I_1 I_2 = 1) - Pr(I_1 = 1)Pr(I_2 = 1)\Big],$$

$$Pr(I_1 = 1) = \frac{\begin{pmatrix} 1 \\ 1 \end{pmatrix}\begin{pmatrix} N-1 \\ n-1 \end{pmatrix}}{\begin{pmatrix} N \\ n \end{pmatrix}} = \frac{n}{N},$$

$$Pr(I_1 = 1)Pr(I_2 = 1) = \frac{\begin{pmatrix} 2 \\ 2 \end{pmatrix}\begin{pmatrix} N-2 \\ n-2 \end{pmatrix}}{\begin{pmatrix} N \\ n \end{pmatrix}} = \frac{n(n-1)}{N(N+1)}.$$

Then,

$$\frac{mn}{N}\frac{(N-n)}{N} + 2\begin{pmatrix} M \\ 2 \end{pmatrix}\left[\frac{n(n-1)}{N(N-1)} - \frac{n^2}{N^2}\right] = n\begin{pmatrix} M \\ N \end{pmatrix}\left(1 - \frac{M}{N}\right)\left(\frac{N-n}{N-1}\right) = Var(x).$$

13.15 Binomial, Negative Binomial, and Multivariate Distributions

Consider an experiment with two possible outcomes (mutually exclusive and exhaustive) which for purposes of identification will be called *success* and *failure.* Let $p = P(\text{success})$ and $1-p = P(\text{failure}), 0 \le p \le 1$. Define a random variable x to be the number of successes in n independent trials of the experiment. x is called the *binomial* random variable with parameters n, p. Clearly, x is discrete with space $0, 1, ..., n$. The density of x is

$$f(x) = \begin{cases} \begin{pmatrix} n \\ x \end{pmatrix} p^x(1-p)^{n-x}, & x = 0, 1, .., n. \\ 0, & \text{otherwise.} \end{cases}$$

To verify this is a density, recall the binomial formula.

$$(a+b)^n = \sum_{x=0}^{n} \begin{pmatrix} n \\ x \end{pmatrix} a^x b^{n-x}$$

where a, b are any two real numbers and n is an integer. So,

$$\sum_{x=0}^{n} f(x) = \sum_{x=0}^{n} \begin{pmatrix} n \\ x \end{pmatrix} p^x(1-p)^{n-x} = [p + (1-p)]^n = 1^n = 1.$$

The mgf of x is

$$M(t) = E(e^{tx}) = \sum_{x=0}^{n} \begin{pmatrix} n \\ x \end{pmatrix} p^x(1-p)^{n-x}e^{tx} = \sum_{x=0}^{n} \begin{pmatrix} n \\ x \end{pmatrix} (pe^t)^x(1-p)^{n-x} = [pe^t+1-p]^n = [1-p+pe^t]^n.$$

The text book uses this to get μ and σ^2. We calculate directly,

$$E(x) = \sum_{x=0}^{n} xf(x) = \sum_{x=0}^{n} x \begin{pmatrix} n \\ x \end{pmatrix} p^x(1-p)^{n-x} = \sum_{x=1}^{n} x\frac{n!}{x!((n-x)!}p^x(1-p)^{n-x} =$$

$$\sum_{x=1}^{n} \frac{n!}{(x-1)!(n-x)!}p^x(1-p)^{n-x} = n\sum_{x=1}^{n} \begin{pmatrix} n-1 \\ x-1 \end{pmatrix} p^x(1-p)^{n-x} = np\sum_{x=1}^{n} \begin{pmatrix} n-1 \\ x-1 \end{pmatrix} p^{x-1}(1-p)^{n-x}.$$

Let $y = x - 1$, then,

$$np\sum_{y=0}^{n-1} \begin{pmatrix} n-1 \\ y \end{pmatrix} p^y(1-p)^{n-1-y} = np.$$

$$E(x^2) = \sum_{x=0}^{n} x^2 \begin{pmatrix} n \\ x \end{pmatrix} p^x(1-p)^{n-x} = \sum_{x=1}^{n} x^2\frac{n!}{x!(n-x)!}p^x(1-p)^{n-x} =$$

$$\sum_{x=1}^{n} \frac{xn!}{(x-1)!(n--x)!}p^x(1-p)^{n-x} = np\sum_{y=0}^{n-1}(y+1) \begin{pmatrix} n-1 \\ y \end{pmatrix} p^y(1-p)^{n-1-y} = np[(n-1)p+1]. \Rightarrow$$

$$Var(x) = np[(n-1)p + 11] - n^2p^2 = np\{np - p + 1 - np\} = np(1-p),$$

where $y = x - 1 = E(y+1)$ where y is $bin(n-1, p)$. Let,

$$f(x) = \begin{cases} \begin{pmatrix} n \\ x \end{pmatrix} p^x(1-p)^{n-x}, & x = 0, 1, 2, ..., n. \\ 0, & \text{otherwise.} \end{cases}$$

The special case of $n = 1$ is called the *Bernoulli Distribution* (which we encountered previously as the distribution of an indicator variable). For $n = 1$,

$$f(x) = \left.\begin{pmatrix} 1 \\ x \end{pmatrix} p^x(1-p)^{1-x}, x = 0, 1\right\} = \begin{cases} 1-p, & x = 0. \\ p, & x = 1. \end{cases}$$

Clearly, the Binomial is the number of successes in n independent Bernoulli trials: $x = \sum_{j=1}^{n} I_j$ where I_j is an indicator that trial j is a success, $x \sim b(n, p)$.

Example: Draw n cards from a standard deck of cards with replacement. Let x be the number that are Jack, Queen, King, and Ace. $p = \frac{4}{13} = \frac{16}{52}$ With $n = 3$,

$$P(\text{Jack or better}) = \frac{4}{3}\left(\frac{4}{13}\right)^2\left(\frac{9}{13}\right)^1$$

A different random variable is defined as follows. We fix the number of successes, r, and ask how many independent trials before the $r-th$ success occurs. Let y be the total number of failures before success r. $y + r$ is the number of trials to produce the $r-th$ success. Let's derive the distribution of y.

$$P(Y = y) = P(r-1 \text{ successes on 1st } y + r - 1 \text{ trials and } (y+r)\text{th try success}) =$$

$$P(r-1 \text{ success on 1st } y+r-1 \text{ trys}) \times P(\text{success on try } y+r) = \begin{pmatrix} y+r-1 \\ r-1 \end{pmatrix} p^{r-1}(1-p)^{y+r-1}p =$$

$$\begin{cases} \begin{pmatrix} y+r-1 \\ r-1 \end{pmatrix} p^r(1-p)^{y+r-1} & y = 0, 1, 2, ... \\ 0, & \text{otherwise.} \end{cases}$$

y is called the *negative binomial* random variable. The special case of $r = 1$ is called the *geometric distribution.*

$$g(y) = \begin{cases} p(1-p)^y, & y = 0, 1, 2, ... \\ 0, & \text{otherwise.} \end{cases}$$

Now we generalize the binomial. Suppose an experiment can result in 1 of k mutually exclusive and exhaustive outcomes: $c_1, c_2, ..., c_k$. $c_i \cap c_j = \emptyset, \cup c_i = \Omega$. Let

$$p_i = P(c_i) \Rightarrow \sum_{i=1}^{k} p_i = 1.$$

We will perform n independent trials of this experiment and count $x_1, x_2, ..., x_{k-1}$ where x_i is the number of the n trials that result in c_i. For any $x_1, x_2, ..., x_{k-1} \ni$: $\sum_{i=1}^{k-1} x_i \leq n$ and $x_i \geq 0, c = 1, 2, ..., k-1$.

$$Pr(X_1 = x_1, X_2 = x_2, ..., X_{k-1} = x_{k-1}) = \frac{n!}{x_1!x_2!x_{k-1}!(n - \sum_{i=1}^{k-1})!} c_1 c_2 \cdots c_{k-1} c_k$$

where

$$c_1 = p_1^{x_1}, c_2 = p_2^{x_2}, ..., c_{k-1} = p_{k-1}^{x_{k-1}}, c_k = \left(1 - \sum_{i=1}^{k-1} p_i^{(n - \sum_{i=1}^{k-1} x_i)}\right)$$

$$p_1^{x_1} p_2^{x_2} \cdots p_{k-1}^{x_{k-1}} \left(1 - \sum_{i=1}^{k-1} p_i^{(n - \sum_{i=1}^{k-1} x_i)}\right) = \frac{n!}{x_1!x_2! \cdots x_k!} p_1^{x_1} p_2^{x_2} \cdots p_k^{x_k},$$

$$x_k = n - \sum_{i=1}^{k-1} x_i.$$

This is called the *multivariate density.* For the special case $k = 2$

$$Pr(X_1 = x_1) = \frac{n!}{x_1!(n - x_1)!} p_1^{x_1} (1 - p_1^{n - x_1})$$

is the *binomial distribution.* It is the pdf for the *multinomial distribution* of $(x_1, x_2, ..., x_{k-1})$. When $k = 3$, it is called the *trinomial distribution.* The density is

$$Pr(X_1 = x_1, X_2 = x_2, X_3 = x_3) = \begin{cases} \frac{n!}{x_1!x_2!x_3!} p_1^{x_1} p_2^{x_2} p_3^{x_3}, & x_1 \geq 0, x_2 \geq 0, x_3 \geq 0. \\ 0, & \text{otherwise.} \end{cases}$$

$x_1 + x_2 + x_3 = n, x_i \geq 0.$

Example: Take n draws with replacement from a standard deck of cards. Define the following random variables: x_1 = number of aces. x_2 = number of kings. x_3 = number of queens and jacks. x_4 = number of 10's, 9's, and 8's. For $k = 5$:

$$p_1 = \frac{1}{13}, p_2 = \frac{1}{13}, p_3 = \frac{2}{13}, p_4 = \frac{3}{13}, p_5 = 1 - \sum_{i=11}^{4} p_i = \frac{6}{13}.$$

For $n = 10$:

$$Pr(x_1 = 2, x_2 = 1, x_3 = 2, x_4 = 4) = \frac{10!}{2!1!2!4!1!} \left(\frac{1}{13}\right)^2 \left(\frac{1}{13}\right)^1 \left(\frac{2}{13}\right)^2 \left(\frac{3}{13}\right)^4 \left(\frac{6}{13}\right)^1.$$

The following results can be established for the multinomial: (see homework later on):

1. The distribution of any subset of $x_1, x_2, ..., x_{k--1}$ is also multinomial.

2. Conditionals are multinomial.

13.16 The Poisson Distribution

Recall that:

$$\sum_{x=0}^{\infty} \frac{m^x}{x!} = e^m \text{ (for any } m).$$

Hence,

$$f(x) = \begin{cases} \frac{m^x e^{-m}}{x!}, & x = 0, 1, 2, ... \\ 0, & \text{otherwise.} \end{cases}$$

is the density for a discrete random variable. Such a random variable is said to have a *Poisson Distribution.* This distribution is empirically known to accurately model many discrete time processes, i.e. the number of occurences of some phenomenon within a given time period interval. In fact, with appropriate assumptions, this density can be derived for such a situation:

1. The chance of one occurrence in a time interval is proportional to the length of the interval.
2. The chance of more than one occurences is proportional to the number of small intervals.
3. Disjoint intervals are independent.

See the Remark on pages 126-128 of the text book. We derive the mgf:

$$M(t) = E(e^{tx}) = \sum_{x=0}^{\infty} \frac{e^{tx} m^x e^{-m}}{x!} =$$

$$e^{-m} \sum_{x=0}^{\infty} \frac{(e^t m)^x}{x!} = e^{-m} e^{e^t m} = exp\{m(e^t - 1)\}.$$

$$\frac{\partial}{\partial t} M(t) = me^t M(t)\Big|_{t=0} = M(0)me^0 = m.$$

$$\frac{\partial^2}{\partial t^2} M(t) = m\{M(t)me^t + M(t)e^t\}_{t=0}.$$

$$m(m+1) = m^2 + m = E(x^2).$$

$$Var(x) = m^2 + m - m^2 = m.$$

Since $m = \mu$, it is common to write

$$f(x) = \begin{cases} \frac{\mu^x e^{-\mu}}{x!}, & x = 0, 1, 2, ... \\ 0, & \text{elsewhere.} \end{cases}$$

13.17 The Gamma Distribution

For $\alpha > 0$, define the *gamma distribution* as:

$$\Gamma(\alpha) = \int_0^\infty y^{\alpha-1} e^{-y}\, dy.$$

Note that $\Gamma(\alpha) = (\alpha-1)\Gamma(\alpha-1)$.

$$\int_0^\infty y^{\alpha-1} e^{-y}\, dy.$$

Let $u = y^{\alpha-1}$. Then using calculus,

$$\int v = e^{-y}, \quad du = (\alpha-1)y^{\alpha-2}\, dy, \;\; v = e^{-y}.$$

$$\overbrace{-y^{\alpha-1}e^{-y}\Big|_0^\infty}^{=0} + \int_0^\infty (\alpha-1)y^{\alpha-2}e^{-y}\, dy = (\alpha-1)\int_0^\infty y^{\alpha-2}e^{-y}\, dy = (\alpha-1)\Gamma(\alpha-1).$$

For $\Gamma(1) = 1$,

$$\Gamma(\alpha) = (\alpha-1)\Gamma(\alpha-1) = (\alpha-1)(\alpha-2)\Gamma(\alpha-1) = (\alpha-1)(\alpha-2)\cdots 2\Gamma(1) \text{ if } \alpha \text{ is an integer} = (\alpha-1)!$$

In the integral, let $x = \beta y$ for some $\beta > 0$. Then,

$$y = \frac{x}{\beta}, \quad dy = \frac{1}{\beta}\, dx,$$

$$\Gamma(\alpha) = \int_0^\infty \left(\frac{x}{\beta}\right)^{\alpha-1} e^{-\frac{x}{\beta}} \frac{1}{\beta}\, dx$$

or

$$1 = \frac{1}{\Gamma(\alpha)\beta^\alpha} \int_0^\infty x^{\alpha-1} e^{-x\beta}\, dx.$$

Definition: A random variable has a *gamma distribution* with parameters $\alpha > 0$ and $\beta > 0$ if it's pdf is

$$f(x) = \begin{cases} \frac{1}{\Gamma(x)\beta^\alpha} x^{\alpha-1} e^{-\frac{x}{\beta}}, & x > 0. \\ 0, & \text{otherwise.z} \end{cases}$$

Definition: The *Gamma function is*

$$\Gamma(\alpha) = \int_0^\infty x^{\alpha-1} e^{-x}\, dx.$$

If α is an integer, then $\Gamma(\alpha) = (\alpha-1)!$

Definition: The Gamma Distribution has the density

$$f(x) = \begin{cases} \frac{1}{\Gamma(x)\beta^\alpha} x^{\alpha-1} e^{-\frac{x}{\beta}}, & x > 0. \\ 0, & x \leq 0. \end{cases}$$

where $\alpha > 0$ and $\beta > 0$. The mgf for the Gamma distribution is

$$M(t) = E(e^{tx}) = \int_0^\infty \frac{e^{x(t-\frac{1}{\beta})}}{\Gamma(\alpha)\beta^\alpha} = x^{-\alpha-1}\, dx = \frac{1}{\beta^\alpha} \int_0^\infty \frac{1}{\Gamma(\alpha)} e^{-\frac{1}{\beta}(1-\beta t)x} x^{\alpha-1}\, dx =$$

$$\frac{1}{\beta^\alpha} \left[\frac{\beta}{1-\beta t}\right]^\alpha \int_0^\infty \frac{1}{\Gamma(\alpha)(\frac{\beta}{1-\beta t})^\alpha} e^{-\frac{x}{\beta/(1-betat)}} x^{\alpha-1}\, dx$$

The integral part is the gamma density with parameters α and $\frac{\beta}{1-\beta t}$ where

$$\frac{\beta}{1-\beta t} > 0 \Rightarrow \beta t < 1 \Rightarrow t < \frac{1}{\beta} = (1-\beta t)^{-\alpha}, t < \frac{1}{\beta},$$

$$M(t) = (1-\beta t)^{-\alpha}, |t| < \frac{1}{\beta},$$

$$E(x) = \frac{\partial}{\partial t} M(t)\bigg|_{t=0} = -\alpha(1-\beta t)^{-\alpha-1}(-\beta) = \alpha\beta(1-\beta t)^{-\alpha-1}.$$

Given,

$$M'(0) = \alpha\beta,$$

$$E(x^2) = \frac{\partial^2}{\partial t^2} M(t)\bigg|_{t=0} = -\alpha\beta(\alpha+1)(1-\beta t)^{-\alpha-2}(-\beta)\bigg|_{t=0}.$$

$$\Rightarrow M''(0) = \alpha\beta^2(\alpha+1), \Rightarrow Var(x) = \alpha(\alpha+1)\beta^2 - \alpha^2\beta^2 = \alpha^2\beta^2 + \alpha\beta^2 - \alpha^2\beta^2 = \alpha\beta^2.$$

When $\alpha = 1$, the gamma distribution is called the *exponential distribution.*

$$f(x) = \begin{cases} \frac{1}{\beta} e^{-\frac{x}{\beta}}, & x > 0. \\ 0, & \text{otherwise.} \end{cases}$$

The mgf is $M(t) = \frac{1}{1-\beta t}$. It is sometimes written with $(\lambda = \frac{1}{\beta})$ as

$$f(x) = \begin{cases} \lambda e^{-\lambda x}, & x > 0. \\ 0, & \text{otherwise.} \end{cases}$$

The new mgf is $M(t) = \frac{\lambda}{\lambda - t}$. Another special case arises when $\alpha = \frac{r}{2}$, where r is an integer and $\beta = 2$. This is called the *Chi-square distribution* denoted by

$$f(x) = \begin{cases} \frac{1}{\Gamma(\frac{1}{2})2^{\frac{r}{2}}} x^{\frac{r}{2}-1} e^{-\frac{x}{2}}, & x > 0. \\ 0, & \text{otherwise.} \end{cases}$$

r is called the *degrees of freedom.* The moment generating function is $M(t) = (1-2t)^{-\frac{r}{2}}, |t| < \frac{1}{2}$.

Example: Bad luck at banks. Person A and Person B enter the bank and join separate lines of equal length simultaneously. Let x be the time til service for Person A, and y be the time til service for Person B. x and y are independent with the same exponential distribution. Consider $\frac{x}{y}$.

$$f(x,y) = \begin{cases} \lambda^2 e^{-\lambda(x+y)}, & x > 0, y > 0. \\ 0, & \text{otherwise.} \end{cases}$$

$$Pr(\text{Person A waits at least 3 times as long as Person B}) = Pr\left(\frac{x}{y} > 3\right) = \int_0^\infty \int_{3y}^\infty \lambda^2 e^{-\lambda(x+y)}\, dx\, dy =$$

$$\int_0^\infty \lambda e^{-\lambda y} \left(-e^{-\lambda x}\right)_{3y}^\infty dy = \int_0^\infty \lambda e^{-\lambda y} e^{-3\lambda y}\, dy = \int_0^\infty \lambda e^{-4\lambda y}\, dy = \frac{1}{4} \overbrace{\int_0^\infty 4\lambda e^{-4\lambda y}\, dy}^{=1} = \frac{1}{4}.$$

Given the same problem, what is the expected ratio?

$$E\left(\frac{x}{y}\right) = \int_0^\infty \int_0^\infty \frac{x}{y} e^{-\lambda(x+y)}\, dx\, dy = \int_0^\infty \lambda \frac{1}{y} e^{-\lambda y} \overbrace{\int_0^\infty \lambda x e^{-\lambda x}\, dx}^{=\frac{1}{\lambda}}\, dy,$$

with $\alpha = 1$, and $\beta = \frac{1}{\lambda}$,

$$\int_0^\infty \frac{1}{y} e^{-\lambda y}\, dy = \int_0^1 \frac{1}{y} e^{-\lambda y}\, dy + \int_1^\infty \frac{1}{y} e^{-\lambda y}\, dy \geq \int_1^\infty \frac{1}{y} e^{-\lambda y}\, dy + \int_0^1 \frac{1}{y} e^{-\lambda}\, dy = e^{-\lambda} \log y \Big|_0^1 \geq 0 + \cdots = \infty + \geq 0.$$

In other words $E(\frac{x}{y}) = \infty$. The *Beta Distribution:* For $\alpha > 0$, and $\beta > 0$ define the *Beta function* by

$$B(\alpha, \beta) = \int_0^1 y^{\alpha-1}(1-y)^{\beta-1}\, dy.$$

Then,

$$f(x) = \begin{cases} \frac{1}{B(\alpha,\beta)} x^{\alpha-1}(1-x)^{\beta-1}, & 0 < x < 1. \\ 0, & \text{otherwise.} \end{cases}$$

is a density for a continuous random variable. Such a random variable is said to have a *Beta Distribution.*

Fact: $B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}$. (this will be proven in chapter 4 of the text book). This allows for easy calculation of the moments of the Beta Distribution.

$$E(x^k) = \frac{1}{B(\alpha,\beta)} \int_0^1 x^k x^{\alpha-1}(1-x)^{\beta-1}\, dx = \frac{B(\alpha+k,\beta)}{B(\alpha,\beta)} \overbrace{\frac{1}{B(\alpha+k,\beta)} \int_0^1 x^{(\alpha+k)-1}(1-x)^{\beta-1}\, dx}^{=1} =$$

$$\frac{\Gamma(\alpha+k)\Gamma(\beta)}{\Gamma(\alpha+k\beta)}\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} = \frac{\Gamma(\alpha+k)}{\Gamma(\alpha+k\beta)}\frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)}.$$

Note that

$$\Gamma(\alpha) = (\alpha-1)\Gamma(\alpha-1) \Rightarrow \frac{(\alpha+k-1)(\alpha+k-2)(\alpha+k-3)\cdots\alpha}{(\alpha+\beta+k-1)(\alpha+\beta+k-2)\cdots(\alpha+\beta)}.$$

So, for $k=1, \Rightarrow E(x) = \frac{\alpha}{\alpha+\beta}$. For $k=2$,

$$\Rightarrow E(x^2) = \frac{(\alpha+1)\alpha}{(\alpha+\beta+1)((\alpha+\beta)} \Rightarrow Var(x) = \frac{\alpha(\alpha+1)}{(\alpha+\beta)(\alpha+\beta+1)} - \frac{\alpha^2}{(\alpha+\beta)^2} = \frac{\alpha\beta}{(\alpha+\beta)^2(\alpha+\beta+1)}.$$

Special Case: When $\alpha=\beta=1$, the Beta Distribution is called the *Uniform Distribution.* The density is

$$f(x) = \begin{cases} 1, & 0<x<1. \\ 0, & \text{otherwise.} \end{cases}$$

$$E(x) = \frac{1}{2},\ \ Var(x) = \frac{1}{12}.$$

13.18 The Normal Distribution

We have from calculus (or page 138 of the text book):

$$\int_{-\infty}^{\infty} e^{-\frac{1}{2}y^2}\,dy = \sqrt{2\pi}.$$

Let $x = a+by$ where $b>0$. Then, $y = \frac{x-a}{b}$, and $dy = \frac{1}{b}\,dx$. Then,

$$\int_{-\infty}^{\infty} \frac{e^{-\frac{1}{2}\frac{(x-a)^2}{b^2}}}{b\sqrt{2\pi}}\,dx = 1.$$

Definition: A random variable has a *Normal Distribution* with parameters a,b if its density is

$$f(x) = \begin{cases} \frac{1}{b\sqrt{2\pi}}e^{-\frac{1}{2}\frac{(x-a)^2}{b^2}}, & -\infty<x<\infty. \end{cases}$$

Let's find the mgf:

$$E(e^{tx}) = \frac{1}{\sqrt{2\pi}}\frac{1}{b}\int_{-\infty}^{\infty} e^{tx}e^{-\frac{1}{2}\frac{(a-b)^2}{b^2}}\,dx = \frac{1}{\sqrt{2\pi}}\frac{1}{b}\int_{-\infty}^{\infty} e^{-\frac{1}{2b^2}[x^2-2ax+a^2-2b^2tx]}\,dx =$$

$$\frac{1}{b}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2b^2}[x^2-2ax+a^2-2b^2tx]}\,dx = \frac{1}{b}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2b^2}[(x-(a+b^2t))^2+a^2-(a+b^2t)^2]}\,dx =$$

$$e^{-\frac{1}{2b^2}[-2ab^2t-b^4t^2]}\overbrace{\frac{1}{b\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2b^2}[x-(a+b^2t)]^2}\,dx}^{=1}$$

We have the *Normal Density* with parameters $(a+b^2t)$ and $b=1$. $M(t)=e^{at+\frac{b^2t^2}{2}}$. $E(x)=\frac{\partial}{\partial t}M(t)\Big|_{t=0}=M(t)[a+b^2t]=a+0=a$.

$$E(x^2)=\frac{\partial^2}{\partial^2 t}M(t)\Big|_{t=0}=M(t)[a+b^2t]^2+M(t)b^2\Big|_{t=0}=a^2+b^2\Rightarrow Var(x)=a^2+b^2-a^2=b^2$$

$$\Rightarrow \mu=a,\sigma^2=b^2.$$

Definition(another): A random variable is said to have a *Normal Distribution* with mean μ and variance σ^2 if the density is

$$f(x)=\left\{\ \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}},\quad -\infty<x<\infty.\right.$$

Notation: If $x\sim N(\mu,\sigma^2)$, then the mgf is $e^{(\mu t+\frac{1}{2}\sigma^2t^2)}$

Theorem 1: If x is $N(\mu,\sigma^2)$, then $w=\frac{x-\mu}{\sigma}$ is $N(0,1)$. Proof: The mgf of w is $E(e^{tw})=E(e^{t\frac{(x-\mu)}{\sigma}})=E(e^{\frac{tx}{\sigma}}e^{-\frac{\mu t}{\sigma}})=e^{-\frac{\mu t}{\sigma}}E(e^{\frac{tx}{\sigma}})=e^{-\frac{\mu t}{\sigma}}E(e^{t^*x})$, where $t^*=\frac{t}{\sigma}$. Then, $e^{(-\frac{\mu t}{\sigma}+\frac{\mu t}{\sigma}+\frac{1}{2}\sigma^2\frac{t^2}{\sigma^2})}=e^{\frac{t^2}{2}}$ which is the mgf of $N(0,1)$. Consequences: For any set A, $Pr\left(w\in\frac{A-\mu}{\sigma}\right)=Pr(w\in A^*)$ where A^* is the set A shifted by μ and then all elements divided by σ. $N(0,1)$ is called the *standard normal distribution.*

Theorem 2: If $x\sim N(0,1)$, then $v=\frac{(x-\mu)^2}{\sigma^2}\sim\chi^2(1)$. Proof: Note $v=w^2$ where $w\sim N(0,1)$. The distribution function of $v, v>0$ is $Pr(V\le v)=Pr(w^2\le V)=Pr(-\sqrt{v}\le w\le\sqrt{v})$. by symmetry of $N(0,1)$,

$$2\times Pr(0\le w\le\sqrt{v})=2\frac{1}{\sqrt{2\pi}}\int_0^{\sqrt{v}}e^{-\frac{1}{2}w^2}\,dw$$

Let $y=w^2$, $\Rightarrow w=\sqrt{y}$, $dw=\frac{1}{2\sqrt{y}}\,dy$,

$$\frac{1}{\sqrt{2\pi}}\int_0^v e^{-\frac{1}{2}y}y^{\frac{1}{2}-1}\,dy$$

Then, the density for v is

$$f(x)=\begin{cases}\frac{1}{\sqrt{2\pi}}e^{-\frac{1}{2}y}y^{\frac{1}{2}-1}, & y>0.\\ 0, & y\le 0.\end{cases}$$

which is the *Gamma Density* with $\alpha=\frac{1}{2},\beta=2$, i.e. $\chi^2(1)$.

13.19 Bivariate Normal Distribution

Definition: x,y are bivariate normal random variables if their joint density is

$$f(x,y)=\begin{cases}\frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}}e^{-[-\frac{1}{2(1-\rho^2)}(\frac{x-\mu_1}{\sigma_1})^2-2\rho(\frac{x-\mu_1}{\sigma_1})\frac{(y-\mu_2)}{\sigma_2}+(\frac{y-\mu_2}{\sigma^2})^2]},\\ -\infty<x<\infty,-\infty<y<\infty.\end{cases}$$

We will show several properties of $f(x,y)$ and of the distribution by a certain factorization. Consider inside the []. It can be written

$$\left\{\frac{y-\mu_2}{\sigma_2}-\rho\left(\frac{x-\mu_1}{\sigma_1}\right)\right\}^2+(1-\rho^2)\left(\frac{x-\mu_1}{\sigma_1}\right)^2=\left(\frac{y-bx}{\sigma_2}\right)^2+(1-\rho^2)\left(\frac{x-\mu_1}{\sigma_1}\right)^2$$

where $bx=\mu_2-\rho\frac{\sigma_2}{\sigma_1}(x-\mu_1)$. So,

$$f(x,y)=\frac{1}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}}e-\frac{1}{2(1-\rho^2)}[(\frac{y-bx}{\sigma_2})^2+(1-\rho^2)(\frac{x-\mu_1}{\sigma_1})^2]$$

$$=\overbrace{\frac{1}{\sigma_1\sqrt{2\pi}}e^{-\frac{1}{2}\frac{(x-\mu_1)^2}{\sigma_1^2}}}^{\text{Density for } N(\mu_1,\sigma_1^2)}\times\overbrace{\frac{1}{\sigma_2\sqrt{2\pi}}e^{-\frac{1}{2}(\frac{y-bx}{\sqrt{1-\rho^2}\sigma_2})^2}\frac{1}{\sqrt{1-\rho^2}}}^{\text{for fixed } x,\ N(bx,(1-\rho^2)\sigma_2^2)}$$

Therefore,

1.
$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}f(x,y)\,dy\,dx=$$

$$\int_{-\infty}^{\infty}\frac{1}{\sigma_1\sqrt{2\pi}}e^{-\frac{1}{2}\frac{(x-\mu_1)^2}{\sigma_1^2}}\,dx\overbrace{\int_{-\infty}^{\infty}\frac{1}{\sigma_2\sqrt{2\pi}}e^{-\frac{1}{2}(\frac{y-bx}{\sqrt{1-\rho^2}\sigma_2})^2}\frac{1}{\sqrt{1-\rho^2}}\,dy}^{=1}\int_{-\infty}^{\infty}\frac{1}{\sigma_1\sqrt{2\pi}}e^{-\frac{1}{2}\frac{(x-\mu_1)^2}{\sigma_1^2}}\,dx=1$$

   So, we have verified $f(x,y)$ is a density.

2. From (1),

$$f_1(x)=\int_{-\infty}^{\infty}f(x,y)\,dy=$$

$$\frac{1}{\sigma_1\sqrt{2\pi}}e^{-\frac{1}{2}\frac{(x-\mu_1)^2}{\sigma_1^2}}\overbrace{\int_{-\infty}^{\infty}\frac{1}{\sigma_2\sqrt{2\pi}}e^{-\frac{1}{2}(\frac{y-bx}{\sqrt{1-\rho^2}\sigma_2})^2}\frac{1}{\sqrt{1-\rho^2}}\,dy}^{=1}=\frac{1}{\sigma_1\sqrt{2\pi}}e^{-\frac{1}{2}\frac{(x-\mu_1)^2}{\sigma_1^2}},-\infty<x<\infty.$$

   $x\sim N(\mu_1,\sigma_1^2)$. Likewise, $y\sim N(\mu_2,\sigma_2^2)$.

3. Based on (2), we now see that factorization has this form $f(x,y)=f_1(x)h(x,y)$

$$\Rightarrow h(x,y)=\frac{f(x,y)}{f_1(x)}\Rightarrow h(x,y)=f(y|x)\Rightarrow y|X=x\sim N\left(\overbrace{\frac{\mu_2+\rho\sigma_2(x-\mu_1)}{\sigma_1}}^{bx},\sigma_2^2(1-\rho^2)\right).$$

   Likewise, $X|Y=y\sim N\left(\mu_1+\frac{\rho\sigma_1}{\sigma_2}(y-\mu_2),(1-\rho^2)\sigma_1^2\right)$.

$$M(t_1,t_2)=E(e^{t_1x+t_2y})=\int\int e^{t_1x+t_2y}f(x,y)\,dx\,dy=\int e^{t_1x}f_1(x)\int e^{t_2y}f_2(y|x)\,dy\,dx$$

where

$$\int e^{t_2y}f_2(y|x)\,dy$$

is the mgf of $N(\mu_2+\frac{\rho\sigma_2}{\sigma_1}(x-\mu_1),(1-\rho^2)\sigma_2^2)$.

$$\exp\Big\{\mu_2t_2+\frac{\rho\sigma_2}{\sigma_1}(x-\mu_1)t_2+\frac{1}{2}(1-\rho^2)\sigma_2^2t_2^2\Big\}=$$

$$\exp\Big\{\mu_2t_2+\frac{1}{2}(1-\rho^2)\sigma_2^2t_2^2-\frac{\rho\sigma_2}{\sigma_1}\mu_1t_2\Big\}\times\int\exp\Big\{t_1x+\frac{\rho\sigma_2}{\sigma_1}xt_2\Big\}f_1(x)\,dx=$$

$$\exp\Big\{\mu_2t_2+\frac{1}{2}(1-\rho^2)\sigma_2^2t_2^2-\frac{\rho\sigma_2}{\sigma_1}\mu_1t_2\Big\}\times\overbrace{\int\exp\Big\{(t_1+\frac{\rho\sigma_2}{\sigma_1}t_2)x\Big\}f_1(x)\,dx}^{M(t_1+\frac{\rho\sigma_2t_2}{\sigma_1})}$$

where $M(t)$ is the mgf of $N(\mu_1,\sigma_1^2)$.

$$\exp\Big\{-\frac{\rho\sigma_2}{\sigma_1}\mu_1t_1+\mu_2t_2+\frac{1}{2}(1-\rho^2)\sigma_2^2t_2^2+\mu_1[t_1+\frac{\rho\sigma_2}{\sigma_1}t_2]+\frac{1}{2}\sigma_1^2[t_1+\frac{\rho\sigma_2t_2}{\sigma_1}]^2\Big\}=$$

$$\exp\Big\{\mu_1t_1+\mu_2t_2+\frac{1}{2}(1-\rho^2)\sigma_2^2t_2^2+\frac{1}{2}\sigma_1^2t_1^2+\frac{\sigma_1^2\rho\sigma_2}{\sigma_1}t_1t_2+\frac{1}{2}\frac{\sigma_1^2\rho^2t_2^2}{\sigma_1^2}\Big\}=$$

$$\exp\Big\{(\mu_1t_1+\frac{\sigma_1^2t_1^2}{2})+(\mu_2t_2+\frac{1}{2}\sigma_2^2t_2^2)+\rho\sigma_1\sigma_2t_1t_2\Big\}=M(t_1,0)M(0,t_2)\exp\Big\{\rho\sigma_1\sigma_2t_1t_2\Big\}.$$

Find

$$E(x,y)=\frac{\partial^2}{\partial t_1\partial t_2}M(t_1,t_2)\Big|_{t_1=t_2=0}=\frac{\partial}{\partial t_1}\left\{M(t_1,t_2)[\mu_2+\sigma_2^2t_2+\rho\sigma_1\sigma_2t_1]\Big|_{t_1=t_2=0}\right\}=$$

$$M(t_1,t_2)[\mu_1+\sigma_1^2t_1+\rho\sigma_1\sigma_2t_2][\mu_2+\sigma_2^2t_2+\rho\sigma_1\sigma_2t_1]+M(t_1,t_2)\rho\sigma_1\sigma_2=1[\mu_1][\mu_2]+1\rho\sigma_1\sigma_2.$$

$$\Rightarrow Cov(x,y)=E(xy)-E(x)E(y)=\mu_1\mu_2+\rho\sigma_1\sigma_2-\mu_1\mu_2=\rho\sigma_1\sigma_2.$$

$$\Rightarrow Corr(x,y)=\frac{\rho\sigma_1\sigma_2}{\sigma_1\sigma_2}=\rho.$$

Theorem 3: Let x,y be bivariate normal. Then they are independent iff they are uncorrelated (i.e. iff $\rho=0$). Proof: Independence implies that the correlation is zero. Suppose x,y have $\rho=0$. $M(t_1,t_2)=M(t_1,0)M(0,t_2)$. That implies independence.

13.20 Distribution of Functions of RVs

Let $x_1, x_2, ..., x_n$ be random variables and let $y = u(x_1, x_2, ..., x_n)$ be a function of $x_1, x_2, ..., x_n$.

Definition: A function of one or more random variables that does not depend on any unknown parameter is called a *statistic.*

Example:

1. $y = \sum_{i=1}^{n} \frac{x_i}{n}$ is a statistic called the *sample mean* denoted by $\bar{x}$.

2. $y = \frac{\sum_{i=1}^{n}(x_i - \bar{x})^2}{n}$ is a statistic called the *variance* of the sample and denoted as s^2.

3. $y = \sum_{i=1}^{n}(x_i - E(x_i))^2$ is not a statistic unless each $E(x_i)$ is known.

We generally think of statistics in the following setting: a sample $x_1, x_2, ..., x_n$ of size n from some population has been obtained. For purposes of description, estimating, testing, etc, statistics such as $\bar{x}$ and s^2 are calculated. Often we have a *random sample* defined as follow:

Definition: $x_1, x_2, ..., x_n$ is said to be a *random sample* if they are mutually independent and each x_i has the same distribution.

In practice, selection of $x_i's$ randomly from a given population ensures that the requirements for a random sample hold. Such $x_1, x_2, ..., x_n$ are also said to be iid (identically and independently distributed). In this chapter of the text book, we study the techniques for finding the Distribution of $y = u(x_1, x_2, ..., x_n)$ assuming we know the distribution of $x_1, x_2, ..., x_n$. The simplest (and perhaps least powerful) technique is the *distribution function technique* (used in proof of theorem 2, chapter 3 of the text book). Find the distribution function of $y = G(y) = Pr(Y \leq y) = Pr(u(x_1, x_2, ..., x_n) \leq y)$ and simplify.

Example: (a new proof of Theorem 1, in Chapter 3 of the text book). $x \sim N(0, 1)$, and $y = ax + b$ where $a, b > 0$ are constants. Find the distribution of y.

$$G(y) = Pr(Y \leq y) = Pr(ax + b \leq y) = Pr\left(x \leq \frac{y-b}{a}\right) = \int_{-\infty}^{\frac{y-b}{a}} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}\, dx.$$

Let $y^* = ax + b$. Then, $x = \frac{y^*-b}{a}$, $dx = \frac{1}{a}\, dy^*$, Then,

$$\int_{-\infty}^{y} \frac{1}{\sqrt{2\pi}a} e^{-\frac{1}{2}(\frac{y^*-b}{a})^2}\, dy^*$$

which is the density for $N(b, a^2)$. Then, $y \sim N(b, a^2)$.

13.21 1:1 Transformations

Suppose we have two sets A and B, and the function $u : A \to B$.

Definition: u is 1:1 if $a_1, a_2 \in A, a_1 \neq a_2 \Rightarrow u(a_1) \neq u(a_2)$. i.e. each $a \in A$ has a different image under u.

Definition: u is 'onto' if $b \in B \Rightarrow \exists a \in A \ni: u(a) = b$. i.e. each $b \in B$ is the image of some $a \in A$.

Definition: u is a *1:1 transformation* if it is both 1:1 and onto. In this case, each $a \in A$ is uniquely associated with exactly one $b \in B$ and vice-versa. Likewise, each subset of a is uniquely associated with a subset of B, and vice-versa.

Example: $A = [-1, 1], B = [-3, 3]$, and $u(a) = 3a$ is a 1:1 transformation.

Example: $A = [-1, 1], B = [0, 1]$, and $u(a) = a^2$ is not a 1:1 transformation.

Example: $A = [-1, 1], B = [0, 1]$, and $u(a) = a + 1$ is not unto but a 1:1 transformation.

A lecture is missing here.

Fact: If u is a 1:1 transformation where $\exists w : B \to A \ni w(u(a)) = a, \forall a \in A$ and $u(w(b)) = b, \forall b \in B$, then w is called the *inverse* of u.

13.22 Change of Variables Technique

Example:

$$h(x, y) = \begin{cases} 2(1 - x - y + 2xy), & 0 < x < 1. \\ 0, & \text{otherwise.} \end{cases}$$

Find the distribution of $u = x - y$. Define $w = x$ for the second variable. $\Rightarrow x = w \Rightarrow y = w - u$.

$$J = \begin{vmatrix} 1 & -1 \\ 1 & 0 \end{vmatrix} = 1.$$

$$g(u, w) = h(w, w - u) \times 1 = 2(1 - w - (w - u) + 2w(w - u)) =$$

$$\begin{cases} 2(1 + u - 2wu - 2w + 2w^2), & 0 < w < 1, -1 < u < 1. \\ 0, & \text{otherwise.} \end{cases}$$

$$\begin{matrix} x = w \\ y = w - u \end{matrix} \Rightarrow \begin{matrix} 0 < w < 1 \\ 0 < w - u < 1 \end{matrix} \Rightarrow \begin{matrix} u < w \\ w < u + 1 \end{matrix} \Rightarrow$$

Finally, find the marginal for u.

$$g_1(u) = \int g(u, w)\, dw,$$

if $u < 0$,

$$g_1(u) = \int_0^{1+u} 2(1 + u - 2wu - 2w + 2w^2)\, dw = 2\left(w + uw - w^2u - w^2 + \frac{2w^3}{3}\right)\Bigg|_0^{1+u} =$$

$$2(1 + u + u(1 + u) - (1 + u)^2u - (1 + u)^2 + \frac{2(1 + u)^3}{3}) = \frac{4}{3} + 2u - \frac{2u^3}{3}$$

If $u \geq 0$, then

$$g_1(u) = \int_u^1 g(u, w)\, dw = \int_u^1 2(1 + u - 2wu - 2w + 2w^2)\, dw = \frac{4}{3} - 2u + \frac{2u^3}{3}.$$

Therefore,

$$\begin{cases} \frac{4}{3} + 2u - \frac{2u^3}{3}, & -1 < u < 0. \\ \frac{4}{3} - 2u + \frac{2u^3}{3}, & 0 \le u < 1. \\ 0, & \text{otherwise.} \end{cases}$$

13.23 The Beta, T, and F Distributions

Example: Let x_1, x_2 be independent gamma random variables with the joint density

$$h(x_1, x_2) = \begin{cases} \frac{1}{\Gamma(\alpha)\Gamma(\beta)} x_1^{\alpha-1} x_2^{\beta-1} e^{-x_1-x_2}, & x_1 > 0, x_2 > 0. \\ 0, & \text{otherwise.} \end{cases}$$

Find the marginal distribution of $y_1 = x_1 + x_2$ and $y_2 = \frac{x_1}{x_1+x_2}$. Given that, then solve for x_1 and x_2 : $x_1 = y_1 y_2$, $x_2 = y_1 - y_1 y_2$. Note that the $x's$ are put in terms of the $y's$.

$$J = \begin{vmatrix} y_2 & y_1 \\ 1 - y_2 & -y_1 \end{vmatrix} = -y_1 y_2 - y_1(1 - y_2) = -y_1$$

$$g(y_1, y_2) = h(y_1 y_2, y_1 - y_1 y_2)|-y_1|,$$

$$\begin{matrix} x_1 \ge 0 \\ x_2 \ge 0 \end{matrix} \Rightarrow \begin{matrix} y_1 y_2 > 0 \\ y_1 - y_1 y_2 > 0 \end{matrix} \Leftrightarrow \begin{matrix} y_1 > 0 \\ y_1 > y_1 y_2 \end{matrix} \Rightarrow 1 > y_2 > 0$$

$$g(y_1, y_2) = \frac{1}{\Gamma(\alpha)\Gamma(\beta)} (y_1 y_2)^{\alpha-1} (y_1 - y_1 y_2)^{\beta-1} e^{-y_1} y_1 = \begin{cases} \frac{1}{\Gamma(\alpha)\Gamma(\beta)} y_1^{\alpha+\beta-1} e^{-y_1} y_2^{\alpha-1} (1 - y_2)^{\beta-1}, & y_1 > 0, 0 < y_2 < 1. \\ 0, & \text{otherwise.} \end{cases}$$

Find the marginal densities.

$$g_2(x_2) = \frac{1}{\Gamma(\alpha)\Gamma(\beta)} y_2^{\alpha-1} (1 - y_2)^{\beta-1} \overbrace{\int_0^\infty y_1^{\alpha+\beta-1} e^{-y_1}\, dy_1}^{\Gamma(\alpha+\beta)} = \begin{cases} \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} y_2^{\alpha-1} (1 - y_2)^{\beta-1}, & 0 < y_2 < 1. \\ 0, & \text{otherwise.} \end{cases}$$

which is the Beta distribution.

$$\Rightarrow B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)}.$$

Since y_1 and y_2 are independent,

$$g_1(y_1) = \frac{g(y_1, y_2)}{g_2(y_2)} = \begin{cases} \frac{1}{\Gamma(\alpha+\beta)} y_1^{\alpha+\beta-1} e^{-y_1}, & y_1 > 0. \\ 0, & \text{otherwise.} \end{cases}$$

which is the Gamma distribution with parameters $\alpha + \beta, 1$. Hence,

1. y_1 and y_2 are independent.

2. y_1 is $Gamma(\alpha+\beta,1)$, the sum of two gammas with the second parameter as one is another gamma.
3. y_2 is $Beta(\alpha,\beta)$.
4. It has been proven that $B(\alpha,\beta)=\frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}$.

Example: Let $w\sim N(0,1)$ and $v\sim\chi^2(r)$. Assume that w and v are independent. Find the distribution of $T=\frac{w}{\sqrt{\frac{v}{r}}}$. Let's use $u=v$ for the second variable. Then, $v=u$, $w=T\sqrt{\frac{u}{r}}$,

$$\left|\begin{array}{cc} 1 & 0 \\ \frac{t}{2\sqrt{ru}} & \sqrt{\frac{u}{r}} \end{array}\right| = \sqrt{\frac{u}{r}}.$$

$$h(v,w)=\frac{1}{\sqrt{2\pi}}e^{-\frac{1}{2}w^2}\frac{1}{\Gamma(\frac{r}{2})2^{\frac{r}{2}}}v^{\frac{r}{2}-1}e^{-\frac{v}{2}}, v>0, -\infty<w<\infty.$$

$$g(t,u)=h\left(u,t\sqrt{\frac{u}{r}}\right)\sqrt{\frac{u}{r}}, u>0, -\infty<t<\infty.$$

$$g(t,u)=\frac{1}{\sqrt{2\pi}}\exp\left\{-\frac{1}{2}t^2\frac{u}{r}\right\}\frac{1}{\Gamma(\frac{r}{2})2^{\frac{r}{2}}}u^{\frac{r}{2}-1}e^{-\frac{u}{2}}\sqrt{\frac{u}{r}}=$$

$$\frac{1}{\sqrt{2\pi}\Gamma(\frac{r}{2})2^{\frac{r}{2}}\sqrt{r}}\exp\left\{-\frac{u}{2}\left[\frac{t^2}{r}+1\right]\right\}u^{\frac{r-1}{2}}$$

$$g_1(t)=\frac{1}{\sqrt{2\pi}\Gamma(\frac{r}{2})2^{\frac{r}{2}}}\int_0^u u^{(\frac{r+1}{2})-1}\exp\left\{\frac{-u}{2/(\frac{t^2}{r}+1)}du\right\}=$$

$$\left[\frac{2}{\frac{t^2}{r}+1}\right]^{r+1}\Gamma\left(\frac{r+1}{2}\right)\overbrace{\int_0^\infty\frac{1}{\Gamma(\frac{r+1}{2})[2/(\frac{t^2}{r}+1)]^{\frac{r+1}{2}}}\exp\left\{\frac{2}{\frac{t^2}{r}+1}\right\}du}^{=1}=$$

$$\frac{\Gamma\left(\frac{r+1}{2}\right)}{\Gamma(\frac{r}{2})}\frac{1}{\sqrt{\pi r}}\left(1+\frac{t^2}{r}\right)^{-\frac{r+1}{2}}, -\infty<t<\infty$$

which is the density for the t distribution with r degrees of freedom which arise as a distribution. $N(0,1)$ divided by the square root of an independent χ^2 over it's degrees of freedom.

Example: Let u and v be independent χ^2 random variables with r_1 and r_2 degrees of freedom. The joint density of u,v is

$$h(u,v)=\frac{1}{\Gamma(\frac{r_1}{2})\Gamma(\frac{r_2}{2})2^{\frac{r_1+r_2}{2}}}u^{\frac{r_1}{2}-1}v^{\frac{r_2}{2}-1}e^{-\frac{1}{2}(u+v)}.$$

Find the distribution of

$$F=\frac{\frac{u}{r_1}}{\frac{v}{r_2}}, u>0, v>0.$$

Define, $z = v$, Then, $v = z$, $u = \frac{r_1}{r_2} F z$,

$$J = \begin{vmatrix} 0 & 1 \\ z\frac{r_1}{\sqrt{r_2}} & z\frac{r_1}{r_2} \end{vmatrix} = \left| -z\frac{r_1}{r_2} \right|.$$

$$g(F, z) = h\left(\frac{r_1}{r_2} F z, z\right)\frac{r_1}{r_2} z = \frac{1}{\Gamma(\frac{r_1}{2})\Gamma(\frac{r_2}{2})2^{\frac{r_1+r_2}{2}}}\left(\frac{r_1}{r_2}\right)\left(\frac{r_1}{r_2} F z\right)^{\frac{r_1}{2}-1} z^{\frac{r_2}{2}-1} e^{-\frac{1}{2}z(\frac{r_1}{r_2}F+1)} z,$$

$$\left.\begin{array}{l} \frac{r_1}{r_2} F z > 0 \\ z > 0 \end{array}\right\} \Rightarrow \begin{array}{l} F > 0 \\ z > 0 \end{array}$$

$$= \frac{1}{\Gamma(\frac{r_1}{2})\Gamma(\frac{r_2}{2})2^{\frac{r_1+r_2}{2}}}\left(\frac{r_1}{r_2}\right)^{\frac{r_1}{r_2}} F^{\frac{r_1}{2}-1} z^{\frac{r_1+r_2}{2}-1} \exp\left\{\frac{-z}{[2(\frac{1}{\frac{r_1}{r_2}F+1})]}\right\} \Rightarrow$$

$$g_1(f) = \Gamma(\frac{r_1+r_2}{2})\frac{1}{\Gamma(\frac{r_1}{2})\Gamma(\frac{r_2}{2})2^{\frac{r_1+r_2}{2}}}\left(\frac{r_2}{r_1}\right)^{\frac{r_1}{2}} F^{\frac{r_1}{2}-1} \times \overbrace{\int_0^\infty \frac{z^{\frac{r_1+r_2}{2}-1}}{\Gamma(\frac{r_1+r_2}{2})[\frac{2}{\frac{r_1}{r_2}F+1}]^{\frac{r_1+1}{2}}} e^{-z/2(\frac{1}{\frac{r_1}{r_2}F+1})} dz}^{=1} =$$

$$\begin{cases} \frac{\Gamma(\frac{r_1+r_2}{2})}{\Gamma(\frac{r_1}{2})(\Gamma(\frac{r_2}{2})}\left(\frac{r_1}{r_2}\right)^{\frac{r_1}{2}} F^{\frac{r_1}{2}-1}\left(\frac{r_1}{r_2}F+1\right)^{-\frac{r_1+r_2}{2}}, & F > 0. \\ 0, & \text{otherwise.} \end{cases}$$

which is the density of the F distribution with r_1 and r_2 degrees of freedom.

Fact: If T has a t distribution with r degrees of freedom, then $F = t^2$ has an F distribution with 1 and r degrees of freedom. The proof is left for homework.

13.23.1 Extensions

Let $x_1, x_2, ..., x_n$ be continuous random variables with joint density $h(x_1, x_2, ..., x_n)$ and n dimensional space $A = \{(x_1, ..., x_n)\} \rightarrow: h(x_1, x_2, ..., x_n) > 0$. Let $y_i = u_i(x_1, x_2, ..., x_n), i = 1, 2, ..., n$ with n dimensional space. ß be such that the u_i's are a 1:1 transformation from A to ß. Hence, $\exists w_i, i = 1, 2, .., n$ such that $x_i = w_i(y_1, y_2, ..., y_n)$ and the w_i's are a 1:1 transformation from ß to A. The first partials of the inverse functions are continuous i.e. $\frac{dx_i}{dy_i}$ are continuous for all i, j, and the Jacobian,

$$J = \begin{vmatrix} \frac{dx_1}{dy_1} & \frac{dx_1}{dy_2} & \frac{dx_1}{dy_3} & \cdots & \frac{dx_1}{dy_n} \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ \frac{dx_n}{dy_1} & \frac{dx_n}{dy_2} & \frac{dx_n}{dy_3} & \cdots & \frac{dx_n}{dy_n} \end{vmatrix}$$

$\forall (y_1, y_2, ..., y_n) \in$ ß. Then, the joint density $g(y_1, y_2, ..., y_2)$ of $y_1, y_2, ..., y_n$ is $g(y_1, y_2, ..., y_n) = h(w_1(y_1, ..., y_n)$, $w_2(y_1, ..., y_n)$, ..., $w_n(y_1, ..., y_n))\ |J|$.

Example: Let the random variables x_1, x_2, x_3 be iid $N(0, 1)$. Find the joint density of $y_1 = x_1 + x_2$, $y_2 = x_1 + x_2 + x_3$ and $y_3 = x_1 - x_2$. Then, $x_1 = \frac{y_1+y_3}{2}$, $x_2 = \frac{y_1-y_3}{2}$, $x_3 = y_2 - y_1$. The Jacobian is

$$J = \begin{vmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{2} & 0 & -\frac{1}{2} \\ -1 & 1 & 0 \end{vmatrix} \begin{matrix} \frac{1}{2} & 0 \\ \frac{1}{2} & 0 \\ -1 & 1 \end{matrix} = 0 + 0 + \frac{1}{4} - 0 - -\frac{1}{4} - 0 = \frac{1}{2}.$$

$$h(x_1, x_2, x_3) = \frac{1}{(2\pi)^{\frac{3}{2}}} \exp\left\{-\frac{1}{2}(x_1^2 + x_2^2 + x_3^2)\right\},$$

$$\left.\begin{matrix} -\infty < \frac{y_1+y_3}{2} < \infty \\ -\infty < \frac{y_1-y_3}{2} < \infty \\ -\infty < y_2 - y_1 < \infty \end{matrix}\right\} \Leftrightarrow -\infty < y_i < \infty, i = 1, 2, 3$$

$$\Rightarrow g(y_1, y_2, y_3) = \frac{1}{2} h\left(\frac{y_1 + y_3}{2}, \frac{y_1 - y_3}{2}, y_2 - y_1\right) =$$

$$\frac{1}{2(2\pi)^{\frac{3}{2}}} \exp\left\{-\frac{1}{2}\left(\left(\frac{y_1 + y_3}{2}\right)^2 + \left(\frac{y_1 - y_3}{2}\right)^2 + (y_2 - y_1)^2\right)\right\} =$$

$$\frac{1}{2(2\pi)^{\frac{3}{2}}} \exp\left\{-\frac{1}{2}\left(\frac{y_3^2}{2} + \frac{3y_1^2}{2} - 2y_1y_2 + y_2^2\right)\right\} =$$

$$\frac{1}{\sqrt{2\pi}\sqrt{2}} \exp\left\{-\frac{1}{2}\left(\frac{y_3}{\sqrt{2}}\right)^2\right\} \frac{1}{\sqrt{2}(2\pi)} \exp\left\{-\frac{1}{2}\left(\frac{3y_1^2}{2} - 2y_1y_2 + y_2^2\right)\right\}$$

where

$$\overbrace{\frac{1}{\sqrt{2}(2\pi)} \exp\left\{-\frac{1}{2}\left(\frac{3y_1^2}{2} - 2y_1y_2 + y_2^2\right)\right\}}^{\text{Bivariate Normal}}$$

and

$$\overbrace{\frac{1}{\sqrt{2\pi}\sqrt{2}} \exp\left\{-\frac{1}{2}\left(\frac{y_3}{\sqrt{2}}\right)^2\right\}}^{N(0,1)}.$$

The bivariate normal exponent can be written as

$$-\frac{3}{2}\left[\left(\frac{y_1 - 0}{\sqrt{2}}\right)^2 - \frac{4}{\sqrt{6}}\left(\frac{y_1 - 0}{\sqrt{2}}\right)\left(\frac{y_2 - 0}{\sqrt{3}}\right) + \left(\frac{y_2 - 0}{\sqrt{3}}\right)^2\right].$$

So, put $\sigma_1 = \sqrt{2}, \sigma_2 = \sqrt{3}, \rho = \frac{2}{\sqrt{6}} = \sqrt{\frac{2}{3}}, \mu_1, \mu_2 = 0$. Then it is a bivariate normal.

Example: Let $x_1, x_2, ..., x_n$ be independent and continuous random variables with densities $h_1(x_1), x_1 \in A_1; h_2(x_2), x_2 \in A_2; ...; h_n(x_n), x_n \in A_n$. Define $y_i = u_i(x_i), i = 1, 2, ..., n$ where $u_i, i = 1, 2, ..., n$ is invertible. Then, $x_i = w_i(y_i), i = 1, 2, ..., n$

$$J = \begin{vmatrix} \frac{dw_1}{dy_1} & 0 & 0 & \cdots & 0 \\ 0 & \frac{dw_2}{dy_2} & 0 & \cdots & 0 \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & \frac{dw_n}{dy_n} \end{vmatrix} = \left|\frac{dw_1}{dy_1}\right| \left|\frac{dw_2}{dy_2}\right| \cdots \left|\frac{dw_n}{dy_n}\right|.$$

$$h(x_1, x_2, ..., x_n) = h_1(x_1)h_2(x_2) \cdots h_n(x_n),$$

$$g(y_1, y_2, ..., y_n) = h(w_1(y_1), w_2(y_2), ..., w_n(y_n))|J| =$$

$$h(w_1(y_1))h(w_2(y_2)) \cdots h(w_n(y_n)) \left|\frac{dw_1}{dy_1}\right| \left|\frac{dw_2}{dy_2}\right| \cdots \left|\frac{dw_n}{dy_n}\right|,$$

where $y_1 \in ß_1, y_2 \in ß_2, ..., y_n \in ß_n$, and $ß_i = u_i(a_i)$.

$$h_1(w_1(y_1)) \left|\frac{dw_1}{dy_1}\right| h_2(w_2(y_2)) \left|\frac{dw_2}{dy_2}\right| \cdots h_n(w_n(y_n)) \left|\frac{dw_n}{dy_n}\right|$$

Therefore $y_1, y_2, ..., y_n$ are independent. Functions of independent random variables are also independent. Suppose we want to consider functions which are not 1:1 transformations from A to ß i.e. more than one point of A is mapped to the same point in ß. We can still use the change of variables technique if we can partition A into disjoint subsets $A = \bigcup_{i=1}^{k} A_i$, where the function from A_i to ß is a 1:1 transformation. The new density is

$$g(y_1, y_2, ..., y_n) = \sum_{i=1}^{k} |J_i| h(w_{1i}(y_1, ..., y_n), w_{2i}(y_1, ..., y_n), ..., w_{ni}(y_1, ..., y_n))$$

where $w_{1i}, ..., w_{ni}$ are the inverse of the transformation from A_i to $ß_i$ and J_i is the corresponding Jacobian.

Example:

$$h(x) = \begin{cases} \frac{1}{2}\cos(x), & -\frac{\pi}{2} < x < \frac{\pi}{2}. \\ 0, & \text{otherwise.} \end{cases}$$

$$y = |x|, \;\; A = \left(-\frac{\pi}{2}, \frac{\pi}{2}\right), \;\; ß = \left[0, \frac{\pi}{2}\right].$$

Let

$$A_1 = \left(0, \frac{\pi}{2}\right), \;\; A_2 = \left(-\frac{\pi}{2}, 0\right)$$

Under $A_1 : y = x$, and $x = y, J = 1$. Under $A_2 : y = -x$ and $x = -y, J = -1$.

$$g(y) = \sum_{i=1}^{2} |J_i| h(w_i(y_i)) = \frac{1}{2}\cos(y) + \frac{1}{2}\cos(-y) = \begin{cases} \cos(y), & 0 < y < \frac{\pi}{2}. \\ 0, & \text{otherwise.} \end{cases}$$

13.24 Extension of Substitution of Variables

Suppose we do not have a 1:1 transformation.

Example: Let x_1, x_2 be iid random variables that are $N(0,1)$.

$$h(x_1, x_2) = \frac{1}{2\pi} \exp\left\{-\frac{1}{2}(x_1^2 + x_2^2)\right\}$$

Let $y_1 = x_1^2, y_2 = |x_1+x_2|$. $A = \{(x_1, x_2) \ni: -\infty < x_1 < \infty, -\infty < x_2 < \infty.\}$ ß $= \{(y_1, y_2) \ni: 0 < y_1 < \infty, 0 < y_2 < \infty\}$

Example: $(1,0)$ and $(-1,0)$ map to $(1,1)$. Let $A_1 = (x_1 > 0, x_1 + x_2 > 0)$, $A_2 = (x_1 > 0, x_1 + x_2 < 0)$, $A_3 = (x_1 < 0, x_1+x_2 > 0)$, $A_4 = (x_1 < 0, x_1+x_2 < 0)$. Then, under $A_1 : x_1 = \sqrt{y_1}, x_2 = y_2 - \sqrt{y_1}$, under A_2 : $x_1 = \sqrt{y_1}, x_2 = -y_2 - \sqrt{y_1}$, under $A_3 : x_1 = -\sqrt{y_1}, x_2 = y_2 + \sqrt{y_1}$, under $A_4 : x_1 = -\sqrt{y_1}, x_2 = -y_2 + \sqrt{y_1}$. The Jacobian under A_1 is

$$J_1 = \begin{vmatrix} \frac{1}{2\sqrt{y_1}} & 0 \\ -\frac{1}{2\sqrt{y_1}} & 1 \end{vmatrix} = \frac{1}{2\sqrt{y_1}}, \quad J_2 = J_3 = J_4 = \left|\frac{1}{2\sqrt{y_1}}\right|.$$

$$g(y_1, y_2) =$$

$$\frac{1}{2\pi} \frac{1}{2\sqrt{y_1}} \exp\left\{-\frac{1}{2}\left(y_1 + (y_2 - \sqrt{y_1})^2\right)\right\} + \exp\left\{-\frac{1}{2}(y_1 + (-y_2 - \sqrt{y_1})^2)\right\} +$$

$$\exp\left\{-\frac{1}{2}(y_1 + (y_2 + \sqrt{y_1})^2)\right\} + \exp\left\{-\frac{1}{2}(y_1 + (-y_2 + \sqrt{y_1})^2)\right\} =$$

$$\frac{1}{2\pi} \frac{1}{2\sqrt{y_1}} \left\{2 \exp\left\{-\frac{1}{2}[y_1 + (y_2 - \sqrt{y_1})^2]\right\} + 2 \exp\left\{-\frac{1}{2}[y_1 + (y_2 + \sqrt{y_1})^2]\right\}\right\},$$

$$g(y_1, y_2) = \frac{e^{-\frac{1}{2}y_1}}{2\pi y_1} \left\{\exp\left[-\frac{1}{2}(y_2 - \sqrt{y_1})^2\right] + \exp\left[-\frac{1}{2}(y_2 + \sqrt{y_1})^2\right]\right\}, y_1 > 0, y_2 > 0.$$

13.25 Ordered Statistics

Let $x_1, x_2, ..., x_n$ be iid random variables i.e. they are the random sample. Define $y_1 = \min\{x_1, x_2, ..., x_n\}$ as the *first order statistic.* Define y_2 as the second smallest of $x_1, x_2, ..., x_n$ as the *second order statistic.* Define $y_n = \max(x_1, x_2, ..., x_n)$ as the *n-th order statistic.* Then, $y_1 \leq y_2 \leq \cdots \leq y_n$. We will find the distribution for order statistics. The text book only does the continuous case and for x_i's having finite spaces (A, b). We will derive more generally by the distribution function technique. Consider the distribution function of y_k being the k-th smallest of $x_1, x_2, ..., x_n$. Then,

$$G_k(y_k) = Pr(Y_k \leq y_k) = Pr(\text{at least } k \text{ of the } x\text{'s are} \leq y_k\ ) = \sum_{j=k}^{n} \overbrace{Pr(\text{exactly } j \text{ of the } x\text{'s are} \leq y_k)}^{\text{Binomial probability}}$$

$$\sum_{j=k}^{n} \binom{n}{j} [F(y_k)]^j \left[1 - F(y_k)\right]^{n-j}$$

which is the distribution function of the k-th order statistic. "Success $= x_i \leq y_k$," n trials $= nx_i$'s $Pr(\text{success}) = Pr(x \leq y_k) = F(y_k) =$ distribution function of x. Now suppose we are in the continuous case. Then, we can differentiate $F_k(y_k)$ to get a pdf for y_k.

$$\sum_{j=k}^{n} \binom{n}{j}^{j} [F(y_k)]^{j-1} f(y_k) [1-F(y_k)]^{n-j} + \sum_{j=k}^{n-1} \binom{n}{j} [F(y_k)]^{j} (n-j)[1-F(y_k)]^{n-j-1}[-f(y_k)].$$

Notice that

$$\binom{n}{j}^{j} = \frac{n!j}{j!(n-j)!} = \frac{n!}{(j-1)!(n-j)!} = n\binom{n-1}{y-1}.$$

Notice that

$$\binom{n}{j}(n-j) = \frac{n!(n-j)}{j!(n-j)!} = \frac{n!}{j!(n-j-1)!} = n\binom{n-1}{j}.$$

So,

$$g_k(y_k) = nf(y_k)\left\{\sum_{j=k}^{n}\binom{n-1}{j-1}[F(y_k)]^{j-1}[1-F(y_k)]^{n-j} - \sum_{j=k}^{n-1}\binom{n-1}{j}[F(y_k)]^{j}[1-F(y_k)]^{n-j-1}\right\} =$$

$$nf(y_k)\binom{n-1}{k-1}[F(y_k)]^{k-1}[1-F(y_k)]^{n-k} = \frac{n!}{(k-1)!(n-k)!}f(y_k)[F(y_k)]^{k-1}[1-F(y_k)]^{n-k}, -\infty < y_k < \infty,$$

which is the density for the k-th order statistic (must know this for the exam).

Example: Let n be odd and consider a random sample of size n from a continuous distribution with a distribution function F and the median $m = F^{-1}(\frac{1}{2})$. Find $Pr(y_{\frac{n+1}{2}} < m)$.

$$g_{\frac{n+1}{2}}\left(y_{\frac{n+1}{2}}\right) = \frac{n!f(y_{\frac{n+1}{2}})[F(y_{\frac{n+1}{2}})]^{\frac{n-1}{2}}}{\left(\frac{n-1}{2}\right)!\left(\frac{n-1}{2}\right)!}[1-F(y_{\frac{n+1}{2}})]^{\frac{n-1}{2}} \Rightarrow$$

$$Pr\left(y_{\frac{n+1}{2}} \leq m\right) = \int_{-\infty}^{m} \frac{n!f(y_{\frac{n+1}{2}})[F(y_1\frac{n+1}{2})]^{\frac{n-1}{2}}}{\left(\frac{n-1}{2}\right)!\left(\frac{n-1}{2}\right)!}[1-F(y_{\frac{n+1}{2}})]^{\frac{n-1}{2}}\, dy_{\frac{n+1}{2}}.$$

Let $u = F(y_{\frac{n+1}{2}})$ $du = f(y_{\frac{y+1}{2}})\, dy_{\frac{n+1}{2}}$, Then,

$$\int_0^{\frac{1}{2}} \frac{n!}{\left(\frac{n-1}{2}\right)!\left(\frac{n-1}{2}\right)!}u^{\frac{n-1}{2}}(1-u)^{\frac{n-1}{2}}\, du = \frac{1}{2}\overbrace{\int_0^1 \frac{\Gamma(n+1)}{\Gamma(\frac{n+1}{2})\Gamma(\frac{n+1}{2})}u^{\frac{n+1}{2}-1}(1-u)^{\frac{n+1}{2}-1}\, du}^{=1} = \frac{1}{2}.$$

(looks like a Beta density). In other words,

$$Pr\left(y_{\frac{n+1}{2}} \leq m\right) = \frac{1}{2}.$$

Hence, $y_{\frac{n+1}{2}}$ is called the *sample median.* It has the same median as the original population. Using similar calculations above, for deriving the distribution function $G_k(y_k)$ and the density $g(y_k)$, we can show that the joint density for y_i and y_j in the continuous case is

$$g_{ij}(y_i, y_j) = \frac{n! f(y_i) f(y_j) [F(y_i)]^{i-1}}{(i-1)!(j-i-1)!(n-j)!} [F(y_i) - F(y_j)]^{j-i-1} [1 - F(y_j)]^{n-j}, -\infty < y_i < y_j < \infty$$

(know this on the exam).

Example: Let x_1, x_2, x_3, x_4 be an iid sequence.

$$f(x) = \begin{cases} 2x, & 0 < x < 1. \\ 0, & \text{otherwise.} \end{cases}$$

$$F(x) = \begin{cases} 0, & x \leq 0. \\ x^2, & 0 < x < 0. \\ 1, & x \geq 1. \end{cases}$$

Find the probability that the range of the sample is less than $\frac{1}{2}$. i.e.

$$Pr\left(y_4 - y_1 < \frac{1}{2}\right).$$

Let, $w = y_4 - y_1$, $z = y_4$. Let $w = y_4 - y_1, z = y_4$. Then, $y_1 = z - y, y_4 = z$.

$$J = \begin{vmatrix} -1 & 1 \\ 0 & 1 \end{vmatrix} = -1.$$

$$g_{14}(y_1, y_4) = \frac{4! 2y_1 2y_4}{0!2!0!} [y_4^2 - y_1^2]^2, 0 < y_1 < y_4 < 1.$$

$$f(w, z) = g_{14}(z - w, z)1 = 48(z - w)z[z^2 - (z - w)^2]^2 = 48w^2[4z^4 - 8z^3 w + 5z^2 w^2 - zw^3], 0 < w < z < 1.$$

$$f_1(w) = \int_w^1 f(w, z)\, dz = 48w^2 \left\{ \frac{w^5}{30} - \frac{w^3}{2} + \frac{5w^2}{3} - 2w + \frac{4}{5} \right\}, 0 < w < 1.$$

$$Pr(\text{range} < \tfrac{1}{2}) = \int_0^{\frac{1}{2}} f_1(w)\, dw = \frac{w^8}{5} - 4w^6 + 16w^5 - 24w^4 + \frac{64w^3}{5}\Big|_0^{\frac{1}{2}} = 0.538.$$

13.26 Homework Answers

Answers from Chapter 4 of the text book.

5)

$$G(y) = Pr(Y \leq y) = Pr(-2\ln x^4 \leq y) = Pr\left(\ln x^4 \geq -\frac{y}{2}\right) = Pr(x^4 \geq e^{-\frac{y}{2}}) = Pr(x \geq e^{-\frac{y}{8}}) =$$

$$1 - \int_0^{e^{-\frac{y}{8}}} x\,dx. \cdots \Rightarrow y \sim \chi^2(2).$$

7)

$$Pr\left(\frac{x_1}{x_2} \leq \frac{1}{2}\right) = Pr\left(x_1 \leq \frac{x_2}{2}\right) = \int_0^1 \int_0^{\frac{x_2}{2}} 4x_1x_2\,dx_1\,dx_2 = \int_0^1 2x_1^2x_2\Big|_0^{\frac{x_2}{2}}\,dx_2 =$$

$$\int_0^1 \frac{x_2^2}{2}x_2\,dx_2 = \frac{x_2^4}{8}\Big|_0^1 = \frac{1}{8}.$$

$$Pr\left(x_1x_2 \geq \frac{1}{4}\right) = Pr\left(x_1 \geq \frac{1}{4x_2}\right) = \int_{\frac{1}{4}}^1 \int_{\frac{1}{4x_2}}^1 4x_1x_2\,dx_1\,dx_2 = \cdots$$

13) For $0 < y < 2$:

$$Pr(Y \leq y) = Pr(x_1 + x_2 \leq y) = Pr(x_1 \leq y - x_2) = \int_0^y \int_0^{y-x_2} \frac{1}{4}\,dx_1\,dx_2 = \cdots$$

Must be done for $y > 2$ also.

13)

$$f(x) = \begin{cases} \frac{1}{2}, & 0 < x < 2. \\ 0, & \text{otherwise.} \end{cases}$$

$$f(x_1, x_2) = \begin{cases} \frac{1}{4}, & 0 < x_1 < 2, 0 < x_2 < 2. \\ 0, & \text{otherwise.} \end{cases}$$

$$y = x_1 + x_2,$$

$$G(y) = Pr(Y \leq y) = Pr(x_1 + x_2 \leq y) = \int_{\{x_1+x_2 \leq y\}} \int \frac{1}{4}\,dx_1\,dx_2.$$

```
    x2
    |
  2 |\ x1=y-x2
    | \
    |   \
    |____\__________ x1
          2
```

Case(1): $y < 2$.

$$G(y) = \int_0^y \int_0^{y-x_2} \frac{1}{4}\, dx_1\, dx_2 = \frac{y^2}{8}.$$

Case(2): $2 < y < 4$.

$$1 - \int_{y-2}^{2} \int_{y-x_2}^{2} \frac{1}{4}\, dx_1\, dx_2.$$

$$G(y) = \begin{cases} 0, & y \le 0. \\ \frac{y^2}{8}, & 0 < y \le 2. \\ y - 1 - \frac{y^2}{8}, & 2 < y < 4. \\ 1, & y \ge 4. \end{cases}$$

14)

$$f(x) = \begin{cases} 1, & 0 < x < 1. \\ 0, & \text{otherwise}. \end{cases}$$

$$y = \frac{x_1}{x_2}.$$

$$Pr(Y \le y) = G(y) = Pr\left(\frac{x_1}{x_2} \le y\right) = \int_{\frac{x_1}{x_2} \le y} \int f(x_1, x_2)\, dx_1\, dx_2$$

```
   x2
1  |     / x1 = x2(y)
   |    /
   |   /
   |  /
   | /
   |/____________________________ x1
       1
```

Case (1): $0 < y < 1 \Rightarrow$

$$G(y) = \int_0^1 \int_0^{yx_2} dx_1\, dx_2 = \frac{y}{2}.$$

Case (2): $y > 1 \Rightarrow$

$$G(y) = \int_0^1 \int_{\frac{x_1}{y}}^{1} dx_2\, dx_1 = 1 - \frac{1}{2y} \Rightarrow G(y) = \begin{cases} 0, & y \le 0. \\ \frac{y}{2}, & 0 < y \le 1. \\ 1 - \frac{1}{2y}, & y > 1. \end{cases}$$

$$g(y) = \begin{cases} 0, & y \le 0. \\ \frac{1}{2}, & 0 < y \le 1. \\ \frac{1}{2y^2}, & y > 1. \end{cases}$$

17)

$$Pr(y=2x+1) = Pr\left(\frac{y}{2} = x+1\right) = Pr\left(\frac{y}{2} - 1 = x\right) = \begin{cases} \frac{1}{3}, & y = 3, 5, 7. \\ 0, & \text{otherwise.} \end{cases}$$

19)

$$Pr(y=x^3) = Pr(\sqrt[3]{y} = x) = \begin{cases} \left(\frac{1}{2}\right)^{\sqrt[3]{y}}, & y = 1, 8, 27, ... \\ 0, & \text{otherwise.} \end{cases}$$

25) $y = x^3 \Rightarrow x = \sqrt[3]{y}.$

$$J = \frac{dx}{dy} = \frac{d(y^{\frac{1}{3}})}{dy} = \frac{1}{3}y^{-\frac{2}{3}} = \frac{1}{3y^{\frac{2}{3}}}.$$

$$g(y) = f(y^{\frac{1}{3}})|J| = \frac{y^{\frac{2}{3}}}{9}\frac{1}{3y^{\frac{2}{3}}} = \begin{cases} \frac{1}{27}, & 0 < y < 27. \\ 0, & \text{otherwise.} \end{cases}$$

26) $y = x^2 \Rightarrow 0 < y < \infty, x = y^{\frac{11}{2}}.$

$$J = \frac{dx}{dy} = \frac{1}{2y^{\frac{1}{2}}}.$$

$$g(y) = f(y^{\frac{1}{2}})|J| = \cdots$$

28) $x \sim U\left(-\frac{\pi}{2}, \frac{\pi}{2}\right).$

$$f(x) = \frac{1}{\frac{\pi}{2} + \frac{\pi}{2}} = \begin{cases} \frac{1}{\pi}, & -\frac{\pi}{2} < x < \frac{\pi}{2}. \\ 0, & \text{otherwise.} \end{cases}$$

$$y = \tan x, \;\; x = \tan^{-1} y, \;\; \frac{dx}{dy} = \frac{1}{1+y^2},$$

$$g(y) = f(\tan^{-1} y)\left|\frac{1}{1+y^2}\right| = \left\{\frac{1}{\pi}\left(\frac{1}{1+y^2}\right), -\infty < y < \infty.\right.$$

30) $|J| = -\frac{1}{2}.$

$$h(x_1, x_2) = \frac{1}{2\pi}e^{-\frac{x_1^2}{2} - \frac{x_2^2}{2}}, -\infty < x_1 < \infty, -\infty < x_2 < \infty.$$

$$g(y_1, y_2) = h\left((\frac{1}{2}(y_1+y_2), \frac{1}{2}(y_1-y_2)\right)|J| = \frac{1}{4\pi}e^{-\frac{(y_1+y_2)}{2} - \frac{(y_1-y_2)}{2}}, -\infty < y_1 < \infty, -\infty < y_2 < \infty.$$

Simplify the exponent:

$$-\frac{\frac{1}{4}(y_1^2+2y_1y_2+y_2^2)}{2}-\frac{\frac{1}{4}(y_1^2-2y_1y_2+y_2^2)}{2}=-\frac{\frac{1}{4}(2y_1^2+2y_2^2)}{2}=-\frac{1}{2}\left[\frac{y_1^2}{2}+\frac{y_2^2}{2}\right].$$

Then,

$$g(y_1,y_2)=\frac{1}{4\pi}e^{-\frac{1}{2}[\frac{y_1^2}{2}+\frac{y_2^2}{2}]}$$

$$\frac{1}{\sqrt{4\pi}}e^{-\frac{1}{2}\frac{y_1^2}{2}}\frac{1}{\sqrt{4\pi}}e^{-\frac{1}{2}\frac{y_2^2}{2}}$$

$$\frac{1}{\sqrt{4\pi}}e^{-\frac{1}{2}\left(\frac{y_1}{\sqrt{2}}\right)^2}\frac{1}{\sqrt{4\pi}}e^{-\frac{1}{2}\left(\frac{y_2}{\sqrt{2}}\right)^2}$$

Both are $N(0,2)$ and separable into functions of y_1 and y_2. So, $g(y_1,y_2)=g_1(y_1)g_2(y_2)\Rightarrow$ independence.

44) $T=\frac{w}{\sqrt{\frac{v}{r}}}$; $y=T^2$ is not a 1:1 transformation. $T^2=\frac{w^2}{\frac{v}{r}}=\frac{\frac{u}{1}}{\frac{v}{r}}\sim F(1,r)$, where $u\sim\chi^2(1)$.

46) $y=\frac{1}{1+\frac{r_1}{r_2}w}$, $1+\frac{r_1}{r_2}w=\frac{1}{y}$, $w=\left(\frac{1}{y}-1\right)\frac{r_2}{r_1}$, $\frac{dw}{dy}=-\frac{r_2}{r_1y^2}$.

$$g(y)=f\left(\left[\frac{1}{y}-1\right]\frac{r_2}{r_1}\right)\left|-\frac{r_2}{r_1y^2}\right|=\frac{\Gamma(\frac{r_1+r_2}{2})(\frac{r_1}{r_2})^{\frac{r_1}{2}}}{\Gamma(\frac{r_1}{2})\Gamma(\frac{r_2}{2})}\frac{[(\frac{1}{y}-1)\frac{r_2}{r_1}]^{\frac{r_1}{2}-1}}{[1+\frac{r_1}{r_2}(\frac{1}{y}-1)\frac{r_2}{r_1}]^{\frac{r_1+r_2}{2}}}\frac{r_2}{r_1y^2}=$$

$$\frac{\Gamma(\frac{r_1+r_2}{2})(\frac{1}{y}-1)^{\frac{r_1}{2}-1}}{\Gamma(\frac{r_1}{2})\Gamma(\frac{r_2}{2})(\frac{1}{y})^{\frac{r_1+r_2}{2}}}\frac{1}{y^2}=\cdots$$

116) $E(F)=E\left(\frac{r_2u}{r_1v}\right)=\frac{r_2}{r_1}E(u)E\left(\frac{1}{v}\right)=E(u)=r_1$. So, $E(\frac{u}{r_1})=1$. $E\left(\frac{r_2}{v}\right)=\frac{r_2}{r_2-2}$

1) A stationary train with N cars will be hit by n bombs. Each bomb will hit a car or the place where a previously destroyed car was. Each car (or place) is equally likely to be hit by each bomb, and the bombs are independent of one another. Each bomb destroys all cars that still exist within k cars on either side of the car or place hit ($2k+1<N$). Find the expected number of cars destroyed. HINT: Use indicators. $n=1$.

$$I_j=\begin{cases}1, & \text{if car } j \text{ is destroyed.}\\ 0, & \text{otherwise.}\end{cases}$$

Let x be the number of cars destroyed. Then,

$$E(x)=E\left(\sum_{j=1}^{N}I_j\right)=\sum_{j=1}^{N}Pr(I_j=1),$$

$$Pr(I_1 = 1) = Pr(\text{bomb hits cars } 1, 2, ..., k+1) = \frac{k+1}{N} = Pr(I_N = 1).$$

$$Pr(I_2 = 1) = Pr(I_{N-1} = 1) = \frac{k+2}{N}$$

$$\sum_{j=1}^{N} Pr(I_j = 1) = 2k + 1 - \left(\frac{k^2+k}{N}\right)$$

for 1 bomb ($n = 1$).

$$f(x_1, x_2) = \begin{cases} \frac{x_1 x_2}{36}, & x_1 = 1, 2, 3; x_2 = 1, 2, 3. \\ 0, & \text{otherwise.} \end{cases}$$

$y_1 = x_1 x_2$, $y_2 = x_2$. $ß = \{(y_1, y_2) \in (1,1), (2,2), (3,3), (2,1), (4,2), (6,3), (3,1), (6,2), (9,3)\}$

13.27 Moment Generating Function Technique

Let $y = u(x_1, x_2, ..., x_n)$. Suppose we know the joint density for $x_1, x_2, ..., x_n$ and we want to find the distribution of y. Perhaps we can do this by finding the mgf of y. Calculate

$$E(e^{ty}) = E(e^{tu(x_1,x_2,...,x_n)}) = \int\int \cdots \int e^{tu(x_1,x_2,...,x_n)} f(x_1, x_2, ..., x_n)\, dx_1\, dx_2 \cdots\, dx_n$$

or in the discrete case:

$$\sum\sum \cdots \sum e^{tu(x_1,x_2,...,x_n)} f(x_1, x_2, ..., x_n)$$

Example:

$$f_1(x_1) = \begin{cases} \frac{1}{2}, & x_1 = \pm 1. \\ 0, & \text{otherwise.} \end{cases}$$

$$f_2(x_2) = \begin{cases} \frac{1}{n}, & x_2 = 1, 2, ..., n. \\ 0, & \text{otherwise.} \end{cases}$$

Let x_1, x_2 be independent. $y = x_1 + x_2$,

$$E(e^{ty}) = E(e^{t(x_1+x_2)}) = E(e^{tx_1} e^{tx_2}) = E(e^{tx_1})E(e^{tx_2}) = \left(\frac{e^t + e^{-t}}{2}\right)\left(\frac{1}{n}\sum_{k=1}^{n} e^{tk}\right) =$$

$$\frac{1}{2n}(1 + e^t + e^{tn} + e^{t(n+1)}) + \sum_{k=2}^{n-1} e^{tk} \Rightarrow g(y) = \begin{cases} \frac{1}{2n}, & y = 0, 1, ..., n, n+1. \\ \frac{1}{n}, & y = 2, 3, ..., n-1. \end{cases}$$

Theorem 1: Let $x_1, x_2, ..., x_n$ be mutually independent random variables with $x_i \sim N(\mu_i, \sigma_i^2)$. Then, $y = \sum_{i=1}^{n} k_i x_i$ is $N\left(\sum_{i=1}^{n} k_i \mu_i, \sum_{i=1}^{n} k_i^2 \sigma_i^2\right)$. **Proof:**

$$E(e^{ty}) = E(e^{t\sum k_i x_i}) = E\left(\prod_{i=1}^{n} e^{tk_i x_i}\right)$$

$$\prod_{i=1}^{n} E(e^{tk_i x_i}) = \prod_{i=1}^{n} M_i(tk_i)$$

where $M_i(t)$ is the mgf of x_i.

$$\prod_{i=1}^{n} \exp\left\{\mu_i t k_i + \frac{1}{2}\sigma_i^2 t^2 k_i^2\right\} = \exp\left\{\left(\sum_{i=1}^{n} k_i \mu_i\right) t + \frac{1}{2}\left(\sum_{i=1}^{n} k_i^2 \sigma_i^2\right) t^2\right\}$$

which is the mgf of $N\left(\sum k_i \mu_i, \sum k_i^2 \sigma_i^2\right)$. Notice that this technique works nicely for linear combinations of independent random variables. If $x_1, x_2, ..., x_n$ are independent and $y = \sum_{i=1}^{n} k_i x_i$, then,

$$E(e^{ty}) = E(e^{t\sum k_i x_i}) = \prod_{i=1}^{n} E(e^{tk_i x_i}) = M_i(tk_i).$$

Theorem 2: If $x_1, x_2, ..., x_n$ are independent and x_i has an mgf $M_i(t)$, then $y = \sum_{i=1}^{n} a_i x_i$ has an mgf $\prod_{i=1}^{n} M_i(a_i t)$. Theorem 1 is a special case of Theorem 2.

Theorem 3: Let $x_1, x_2, ..., x_n$ be mutually independent and $x_i \sim \chi^2(r_i)$. Then, $y = \sum_{i=1}^{n} x_i$ is $\chi^2\left(\sum_{i=1}^{n} r_i\right)$.
Proof: By Theorem 2, the mgf of y is

$$M(t) = \prod_{i=1}^{n} (1-2t)^{-\frac{r_i}{2}} = (1-2t)^{-\frac{\sum r_i}{2}}$$

which is the mgf of $\chi^2\left(\sum r_i\right)$.

Theorem 4: Let $x_1, x_2, ..., x_n$ be a random sample from $N(\mu, \sigma^2)$. Then,

$$y = \sum_{i=1}^{n} \left(\frac{x_i - \mu}{\sigma}\right)^2$$

is $\chi^2(n)$. **Proof:** By Theorem 2 of chapter 3 in the text book,

$$\left(\frac{x_i - \mu}{\sigma}\right)^2 \sim \chi^2(1).$$

By the results in section 4.3 in the text book,

$$\left(\frac{x_i - \mu}{\sigma}\right)^2$$

are independent for $i = 1, 2, ..., n$. So, Theorem 3 says the sum is $\chi^2(n)$.

13.28 Distribution of $\bar{x}$ and s^2

Notes:

- $s^2 = \frac{\sum(x_i - \bar{x})}{n}$.
- The square of $N(0,1)$ is $\chi^2(1)$.
- The T statistic is a normal divided by the square root of a chi-square.

The purpose of this section is to prove the following: if $x_1, x_2, ..., x_n$ is a random sample from a normal population $N(\mu, \sigma^2)$, then

1. $\bar{x} \sim N\left(\mu, \frac{\sigma^2}{n}\right)$.
2. $\frac{ns^2}{\sigma^2} = \frac{\sum(x_i - \bar{x})^2}{\sigma^2} \sim \chi^2(n-1)$.
3. $\bar{x}$ and s^2 are independent.

We will prove this by use of moment generating functions. The joint mgf of $\bar{x}, x_1 - \bar{x}, x_2 - \bar{x}, ..., x_n - \bar{x}$ is

$$M(t_0, t_1, ..., t_n) = E\left\{\exp[t_0\bar{x} + t_1(x_1 - \bar{x}) + \cdots + t_n(x_n - \bar{x})]\right\}.$$

The quantity in the exponent is

$$t_0\bar{x} + \sum_{j=1}^{n} t_j x_j - \bar{x}\sum_{j=1}^{n} t_j = \sum_{i=1}^{n}\left(\frac{t_0}{n} + t_i - \bar{t}\right)x_i,$$

where,$\bar{t} = \frac{\sum t_i}{n}$. Write $t_i^* = \frac{t_0}{n} + t_i - \bar{t}$. Then,

$$M(t_0, t_1, ..., t_n) = E\left\{\exp\left[\sum t_i^* x_i\right]\right\}.$$

By Theorem 2,

$$\prod_{i=1}^{n} M_i(t_i^*)$$

where M_i is the mgf of x_i

$$\prod_{i=1}^{n}\exp\left\{\mu t_i^* + \frac{1}{2}\sigma^2 t_i^{*2}\right\} = \exp\left\{\mu\sum t_i^* + \frac{1}{2}\sigma^2\sum t_i^{*2}\right\}.$$

Now, $\sum_{i=1}^{n} t_i^* = 0$ since $n\bar{t} - n\bar{t} = 0$.

$$\sum_{i=1}^{n} t_i^{*2} = \frac{t_0^2}{n} + \sum_{i=1}^{n}(t_i - \bar{t})^2 \Rightarrow M(t_0, t_1, ..., t_n) = \exp\left\{\mu t_0 + \frac{1}{2n}\sigma^2 t_0^2 + \frac{1}{2}\sigma^2\sum(t_i - \bar{t})^2\right\} =$$

$$\overbrace{\exp\left\{\mu t_0 + \frac{1}{2n}\sigma^2 t_0^2\right\}}^{\textit{mgf of } N(\mu, \sigma^2/n).}\exp\left\{\frac{1}{2}\sigma^2\sum(t_i - \bar{t})^2\right\}.$$

And we know from Theorem 1 that $\bar{x} \sim N\left(\mu, \frac{\sigma^2}{n}\right)$. Thus, we have

$$M(t_0, t_1, ..., t_n) = \overbrace{M(t_0, 0, 0, ..., 0)}^{mfg\ of\ \bar{x}} \times \overbrace{M(0, t_1, t_2, ..., t_n)}^{joint\ mgf\ of\ x_1 - \bar{x}, ..., x_n - \bar{x}} \Rightarrow$$

$\bar{x}$ is independent of $x_1 - \bar{x}, ..., x_n - \bar{x}$. $\Rightarrow \bar{x}$ is independent of $s^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$. It remains to show that $\frac{ns^2}{\sigma^2} \sim \chi^2(n-1)$. Easily checked is that

$$\overbrace{\sum_{i=1}^{n}\left(\frac{(x_i - \mu)}{\sigma}\right)}^{\chi^2(n)\ by\ Theorem\ 4} = \overbrace{\frac{ns^2}{\sigma^2}}^{\text{independent}} + \overbrace{\frac{(\bar{x} - \mu)^2}{\sigma^2/n}}^{independent;\chi^2(1).\ Theorem\ 2,\ Chapter\ 3}.$$

Hence, the mgf of the left-hand-side is the product of 2 mgf's for the right-hand-side. $(1-2t)^{-\frac{n}{2}} = M(t)(1-2t)^{-\frac{1}{2}}$ where $M(t)$ is the mgf of $\frac{ns^2}{\sigma^2}$. $\Rightarrow M(t) = (1-2t)^{-\frac{(n-1)}{2}}$ which is the mgf of $\chi^2(n-1)$. $\Rightarrow \frac{ns^2}{\sigma^2} \sim \chi^2(n-1)$.

13.29 Convergence in Distribution

In this chapter we study distributions that depend on an integer n. In particular, we study the distribution as n grows large.

Example: Let $\bar{x}$ be from a normal random sample $\bar{x} \sim N\left(\mu, \frac{\sigma^2}{n}\right)$.

Example: Let x be binomial. The mgf is $(1 - p + pe^t)^n$.

Usually distributions that are a function of n arise from random variables calculated from samples of size n. Sometimes it is difficult to find the distribution for any fixed n, but simplifications arise as $n \to \infty$, for large samples. That is our motivation. If the distribution depends on n, we will indicate this by subscripting the distribution function as $F_n(x)$. For example for $N\left(\mu, \frac{\sigma^2}{n}\right)$,

$$F_n(x) = \int_{-\infty}^{x} \frac{\sqrt{n}}{\sqrt{2\pi}\sigma} e^{-\frac{n}{2}\left(\frac{y-\mu}{\sigma}\right)^2} dy.$$

Definition: Suppose that $\lim_{n\to\infty} F(y) = F(Y)$, at every point y for which F is continuous and suppose further that F is a distribution function. Then, the random variable y_n with the Distribution function $F_n(y)$ is said to have a *limiting distribution* with the distribution function $F(y)$. y_n is said to *converge in distribution* with the distribution function $F(y)$.

Example: If $x_1, x_2, ..., x_n$ are a random sample from a distribution with a density

$$f(x) = \begin{cases} \frac{1}{\theta}, & 0 < x < \theta, \theta > 0 \text{ is fixed.} \\ 0, & \text{otherwise.} \end{cases}$$

$y_n = \max(x_1, x_2, ..., x_n)$. From Chapter 4, the distribution for y_n is

$$F_n(y) = \begin{cases} 0, & y \le 0. \\ \frac{y^n}{\theta^n}, & 0 < y < \theta. \\ 1, & \theta \le y. \end{cases}$$

$$\lim_{n\to n} F_n(y) = \begin{cases} 0, & y \le 0. \\ 0, & 0 < y < \theta. \\ 1, & y \ge \theta. \end{cases}$$

Call this function $F(y)$. It is a distribution function with all its probability on the point θ. y_n converges in distribution to θ.

Example:

$$F_n(y) = \begin{cases} 0, & y \le 0. \\ ny, & 0 < y < \frac{1}{n}. \\ 1, & y \ge \frac{1}{n}. \end{cases}$$

```
  |
  |
1 |     /------------------
  |    /
  |   /
  |  /
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------|------------------------------
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$$\lim_{n\to n} F_n(y) = \begin{cases} 0, & y \le 0. \\ 1, & y > 0. \end{cases}$$

$F_n(y)$ is not a distribution function since it is not right continuous. Manually fit the following distribution:

$$F(y) = \begin{cases} 0, & y < 0. \\ 1, & y \ge 0. \end{cases}$$

to the definition of convergence. Convergence in distribution to the trivial distribution with all probability at zero.

Example: Let $y_n = \max(x_1, x_2, ..., x_n)$, and let $x_1, x_2, ..., x_n$ be iid uniform on $(0, \theta)$. This is the same as the first example. Let $z_n = n(\theta - y_n)$. Then it is easily shown that

$$G_n(z) = \begin{cases} 0, & z < 0. \\ 1 - \left(1 - \frac{z}{n\theta}\right)^n, & 0 \le z \le n\theta. \\ 1, & z \ge n\theta. \end{cases}$$

Remember that

$$\lim_{n\to\infty} \left(1 - \frac{a}{n}\right)^n = e^{-a}.$$

Then,

$$\lim_{n\to\infty} G_n(z) = \begin{cases} 0, & z < 0. \\ 1 - e^{-\frac{z}{\theta}}, & z \ge 0. \end{cases}$$

which is the distribution function of an exponential random variable. Hence z converges in distribution to an exponential distribution.

13.30 Homework Answers

5.2 $f(x) = e^{-(x-\theta)}, \theta < x < \infty$. $z_n = n(y_1 - \theta)$. $g(y_1) = \frac{n! f(y_1)[F(y_1)]^0[1-F(y_1)]^{n-1}}{(1-1)!(n-1)!}$,

$$f(y_1) = e^{-(y_1-\theta)}$$

$$F(y_1) = \int_\theta^{y_1} e^{-(x-\theta)}\,dx = -e^{-(x-\theta)}\Big|_\theta^{y_1} = 1 - e^{-(y_1-\theta)}.$$

$$g(y_1) = ne^{-(y_1-\theta)}[1 - 1 + e^{-(y_1-\theta)}]^{n-1} = ne^{-n(y_1-\theta)}.$$

Let

$$y_1 = \frac{z_n}{n} + \theta \Rightarrow ne^{-n(\frac{z_n}{n}+\theta-\theta)} = ne^{-\frac{nz_n}{n}},$$

$$J = \frac{1}{n},$$

$$|J|g(y_1) = e^{-z_n},$$

$$\int_0^{z_n} e^{-w}\,dw = 1 - e^{-z_n},$$

$$\lim_{n\to\infty} 1 - e^{z_n} = 1.$$

5.3

$$z_n = n[1 - F(y_n)]$$

$$\frac{z_n}{n} = 1 - F(y_n)$$

$$F(y_n) = 1 - \frac{z_n}{n}$$

$$f(y_n) = F' = -\frac{1}{n}$$

$$Pr(Y_n \le y_n) = \frac{n! f(y_n)[F(y_n)]^{n-1}}{(n-1)!(n-n)!} = n[F(y_n)]^{n-1}$$

$$g(y_n) = g\left(1 - \frac{z_n}{n}\right) = |J|f(y_n) = [F(y_n)]^{n-1}.$$

13.31 Homework Answers

49)

$$y_1 = \frac{x_1}{x_1 + x_2},$$

$$y_1(x_1 + x_2) = x_1$$

$$x_1 + x_2 = \frac{x_1}{y_1}$$

$$x_1 - \frac{x_1}{y_1} = -x_2$$

$$x_1\left(1 - \frac{1}{y_1}\right) = -x_2$$

$$x_1 = \frac{-x_2}{1 - \frac{1}{y_1}}$$

$$x_1 = \frac{x_2}{\frac{1}{y_1} - 1} = \frac{y_1 x_2}{1 - y_1}, 0 < y_1 < 1.$$

$$y_2 = \frac{\frac{y_1 x_2}{1-y_1} + x_2}{\frac{y_1 x_2}{1-y_1} + x_2 + x_3}$$

$$y_2\left(\frac{y_1 x_2}{1 - y_1} + x_2 + x_3\right) = \frac{y_1 x_2}{1 - y_1} + x_2$$

$$\frac{y_1 x_2}{1 - y_1} + x_2 + x_3 = \frac{y_1 x_2}{y_2(1 - y_1)} + \frac{x_2}{y_2}$$

$$x_3 = \frac{y_1 x_2}{y_2(1 - y_1)} + \frac{x_2}{y_2} - x_2 - \frac{y_1 x_2}{1 - y_1}, 0 < y_2 < 1.$$

$$y_3 = \frac{y_1 x_2}{y_2(1 - y_1)} + \frac{x_2}{y_2}$$

$$y_3 = \left[\frac{y_1}{y_2(1 - y_1)} + \frac{1}{y_2}\right] x_2$$

$$x_2 = \frac{y_3}{\frac{y_1}{y_2(1-y_1)} + \frac{1}{y_2}} = \frac{y_3 y_2(1-y_1)}{y_1 + 1 - y_1}, y_3 > 0.$$

$$x_2 = y_3 y_2(1-y_1),$$

$$x_1 = y_1 y_2 y_3.$$

$$\frac{1}{1-y_1} y_1 y_2 y_3(1-y_1) + y_2 y_3(1-y_1) + x_3 = \frac{y_1 y_2 y_3(1-y_1)}{y_2(1-y_1)} + \frac{y_2 y_3(1-y_1)}{y_2},$$

$$y_1 y_2 y_3 + y_2 y_3 - y_1 y_2 y_3 + x_3 = y_1 y_3 + y_3 - y_1 y_3,$$

$$x_3 = -y_2 y_3 + y_3.$$

$$g(y_1, y_2, y_3) = e^{-y_1 y_2 y_3} e^{-y_2 y_3(1-y_1)} e^{y_2 y_3 - y_3} = e^{-y_1 y_2 y_3 - y_2 y_3 + y_1 y_2 y_3 + y_2 y_3 - y_3} = e^{-y_3}.$$

$$J = \begin{vmatrix} y_2 y_3 & -y_2 y_3 & 0 \\ y_1 y_3 & y_3(1-y_1) & -y_3 \\ y_1 y_2 & y_2(1-y_1) & 1-y_2 \end{vmatrix} =$$

$$y_2 y_3^2(1-y_1)(1-y_2) + y_1 y_2^2 y_3^2 + 0 - [0 - y_2^2 y_3^2(1-y_1) - (1-y_2) y_1 y_2 y_3^2] =$$

$$[y_2 y_3^2 - y_1 y_2 y_3^2](1-y_2) + y_1 y_2^2 y_3^2 + y_2^2 y_3^2 - y_1 y_2^2 y_3^2 + y_1 y_2 y_3^2 - y_1 y_2^2 y_3^2 = y_2 y_3^2$$

$$\Rightarrow |J| g(y_1, y_2, y_3) = \begin{cases} y_2 y_3^2 e^{-y_3}, & 0 < y_1 < 1, 0 < y_2 < 1, y_3 > 0. \\ 0, & \text{otherwise.} \end{cases}$$

53) $f(x) = \frac{1}{2}, -1 < x < 1$. $y = x^2 \Rightarrow x = \pm\sqrt{y}$. Let $A_1 = (-1 < x < 0), A_2 = (0 < x < 1)$. $A_1 : x = -\sqrt{y}, 0 < y < 1$. $A_2 : x = \sqrt{y}, 0 < y < 1$. $J_1 = -\frac{1}{2\sqrt{y}}$, $J_2 = \frac{1}{2\sqrt{y}}$.

$$g(y) = \frac{1}{2}\frac{1}{2\sqrt{y}} + \frac{1}{2}\frac{1}{2\sqrt{y}} = \begin{cases} \frac{1}{2\sqrt{y}}, & 0 < y < 1. \\ 0, & \text{otherwise.} \end{cases}$$

54) $y_1 = x_1^2 + x_2^2$, $y_2 = x_2$. $y_1 = x_1^2 + y_2^2$, $y_1 - y_2^2 = x_1^2$, $x_1 = \pm\sqrt{y_1 - y_2^2}$, $x_2 = y_2$. $A_1 : (x_1^2 + x_2^2 > 0, x_1 > 0)$, $A_2 : (x_1^2 + x_2^2 > 0, x_1 < 0)$. $A_1 : x_1 = \sqrt{y_1 - y_2^2}, x_2 = y_2$, $A_2 : x_1 = -\sqrt{y_1 - y_2^2}, x_2 = y_2$.

$$J_1 = \begin{vmatrix} \frac{1}{2}(y_1 - y_2^2)^{-\frac{1}{2}} & 0 \\ \frac{1}{2}(-2y_2)(y_1 - y_2^2)^{-\frac{1}{2}} & 1 \end{vmatrix} = \frac{1}{2\sqrt{y_1 - y_2^2}},$$

$$J_2 = \begin{vmatrix} -\frac{1}{2}(y_1 - y_2^2)^{-\frac{1}{2}} & 0 \\ \frac{1}{2}(2y_2)(y_1 - y_2^2)^{-\frac{1}{2}} & 1 \end{vmatrix} = -\frac{1}{2\sqrt{y_1 - y_2^2}}.$$

$$h(x_1, x_2) = \frac{1}{2\pi} e^{-\frac{1}{2}(x_1^2 + x_2^2)},$$

$$g(y_1, y_2) = \frac{1}{2\pi} \frac{e^{-\frac{1}{2}[(y_1 - y_2^2) + y_2^2]}}{2\sqrt{y_1 - y_2^2}} + \frac{1}{2\pi} \frac{e^{-\frac{1}{2}(y_1 - y_2^2 + y_2^2)}}{2\sqrt{y_1 - y_2^2}} =$$

$$\frac{1}{4\pi\sqrt{y_1 - y_2^2}}[e^{-\frac{1}{2}y_1} + e^{-\frac{1}{2}y_1}] = \begin{cases} \frac{1}{2\pi} \frac{e^{-\frac{1}{2}y_1}}{\sqrt{y_1 - y_2^2}}, -\sqrt{y_1} < y_2 < \sqrt{y_1}, 0 < y_1 < \infty. \end{cases}$$

$$g(y_1) = \int_{-\sqrt{y_1}}^{\sqrt{y_1}} \frac{1}{2\pi} \frac{e^{-\frac{1}{2}y_1}}{\sqrt{y_1 - y_2^2}}\, dy_2$$

is the integral of

$$\int \sin^{-1}\left(\frac{y_2}{\sqrt{y_1}}\right)$$

56) $f(x) = e^{-x}$, $f(y_4) = e^{-y_4}$,

$$\int_0^{y_4} e^{-z}\, dx = -e^{-z}\Big|_0^{y_4} = 1 - e^{-y_4} = F(y_4).$$

$$Pr(3 \le y_4) = \frac{4!(e^{-y_4})[1 - e^{-y_4}]^3[1 - 1 + e^{-y_4}]^0}{(3)!(0)!} = 4e^{-y_4}[1 - e^{-y_4}]^3.$$

Integrate from 0 to 3.

62) Find

$$Pr\left(y_4 - y_1 < \frac{1}{2}\right)$$

Let $w = y_4 - y_1, x = y_4$. Then, $z = y_4$, $y_1 = z - w$, $y_4 = z$.

$$J = \begin{vmatrix} -1 & 1 \\ 0 & 1 \end{vmatrix} = -1.$$

$f(x) = 1$. $F(x) = x$, $i = 1, j = 4, n = 4$.

$$g_{1,4}(y_1, y_4) = \frac{4!1 \times 1[y_1]^0[y_4 - y_1]^{4-1-1}[1 - y_4]^0}{0!2!0!} = \begin{cases} 12(y_4 - y_1)^2, & 0 < y_1 < y_4 < 1. \\ 0, & \text{otherwise.} \end{cases}$$

$$f(w, z) = g_{1,4}(z - w, z)1 = 12(z - z + w)^2 = 12w^2, 0 < z - w < z < 1, \text{ or } 0 < w < z < 1.$$

$$f_1(w) = \int_0^1 f(w, z)\,dz = \int_w^1 12w^2\,dz = 12w^2 z\Big|_w^1 = 12w^2 - 12w^3, 0 < w < 1.$$

$$Pr\left(y_4 - y_1 < \frac{1}{2}\right) = \int_0^{\frac{1}{2}} f_1(w)\,dw = \int_0^{\frac{1}{2}} 12w^2 - 12w^3\,dw = \frac{12w^3}{3} - \frac{12w^4}{4}\Big|_0^{\frac{1}{2}} =$$

$$4\frac{1}{8} - 3\frac{1}{16} = \frac{1}{2} - \frac{3}{16} = \frac{5}{16}.$$

78) Given, $x_1 \sim B\left(n_1, \frac{1}{2}\right)$, $x_2 \sim B\left(n_2, \frac{1}{2}\right)$. $y = x_1 - x_2 + n_2$,

$$f_1(x_1) = \begin{cases} \begin{pmatrix} n_1 \\ x_1 \end{pmatrix} \left(\frac{1}{2}\right)^{x_1} (1 - p)^{n_1 - x_1}, & x_1 = 0, 1, , ..., n_1. \\ 0, & \text{otherwise.} \end{cases}$$

$$f_2(x_2) = \begin{cases} \begin{pmatrix} n_2 \\ x_2 \end{pmatrix} \left(\frac{1}{2}\right)^{x_2} \left(\frac{1}{2}\right)^{n_2 - x_2}, & x_2 = 0, 1, , ..., n_2. \\ 0, & \text{otherwise.} \end{cases}$$

$$E(e^{ty}) = E(e^{t(x_1 - x_2 + n_2)}) = E(e^{tx_1})E(e^{t(n_2 - x_2)}),$$

$$E(e^{tx_1}) = \sum_{x_1=0}^{n_1} e^{tx_1} \begin{pmatrix} n_1 \\ x_1 \end{pmatrix} \left(\frac{1}{2}\right)^{x_1} \left(\frac{1}{2}\right)^{n_1 - x_1} = \left[e^t + \frac{1}{2}\right]^{n_1},$$

$$E(e^{t(n_2 - x_2)}) = \sum_{x_2=0}^{n_2} e^{t(n_2 - x_2)} \begin{pmatrix} n_2 \\ x_2 \end{pmatrix} \left(\frac{1}{2}\right)^{x_2} \left(\frac{1}{2}\right)^{n_2 - x_2} =$$

$$\sum_{x_2=0}^{n_2} \begin{pmatrix} n_2 \\ x_2 \end{pmatrix} \left(\frac{1}{2}\right)^{x_2} \left(e^t \frac{1}{2}\right)^{n_2 - x_2} = \left[\frac{1}{2} + \frac{1}{2}e^t\right]^{n_2},$$

$$E(e^{ty}) = \left[\frac{1}{2} + \frac{1}{2}e^t\right]^{n_1 + n_2} \sim Bin\left(n_1 + n_2, \frac{1}{2}\right)$$

81)

$$f_1(x_1) = \begin{cases} \frac{x_1^2 e^{-\frac{x_1}{3}}}{\Gamma(3)3^3}, & x_1 > 0. \\ 0, & \text{otherwise.} \end{cases}$$

$$f_2(x_2) = \begin{cases} \frac{x_2^4 e^{-\frac{x_2}{1}}}{\Gamma(5)1^5}, & x_2 > 0. \\ 0, & \text{otherwise.} \end{cases}$$

$a) y = 2x_1 + 6x_2,$

$$E(e^{ty}) = E(e^{(2x_1+6x_2)t}) = E(e^{2x_1 t})E(e^{6x_x t})),$$

$$E(e^{2x_1 t}) = \int_0^\infty \frac{e^{2x_1 t} x_1^2 e^{-\frac{x_1}{3}}}{\Gamma(3)27}\, dx_1 = \frac{1}{\Gamma(3)27}\int_0^\infty x_1^2 e^{-x_1(\frac{1}{3}-2t)}\, dx_1 =$$

$$\frac{1}{27}\frac{1}{\left(\frac{1}{3}-2t\right)^3}\int_0^\infty \frac{x_1^2 e^{\frac{-x_1}{\frac{1}{(\frac{1}{3}-2t)}}}}{\Gamma(3)(\frac{1}{\frac{1}{3}-2t})^3}\, dx_1 = \frac{1}{27}\left(\frac{1}{\frac{1}{3}-2t}\right)^3 = \frac{1}{27}\left(\frac{3}{1-6t}\right)^3 = \left(\frac{1}{1-6t}\right)^3, |t| < \frac{1}{6}.$$

$$E(e^{6x_2 t}) = \int_0^\infty \frac{e^{6x_2 t} x_2^4 e^{-x_2}}{\Gamma(5)}\, dx_2 = \int_0^1 \frac{x_2^4 e^{-x_2(1-6t)}\, dx_2}{\Gamma(5)}\, dx_2 = \int_0^1 \frac{x_2^4 e^{\frac{-x_2}{\frac{1}{(1-6t)}}}}{\Gamma(5)}\, dx_2,$$

$$\left(\frac{1}{1-6t}\right)^5 \int_0^1 \frac{x_2^4 e^{\frac{-x_2}{\frac{1}{(1-6t)}}}}{\Gamma(5)(\frac{1}{1-6t})^5}\, dx_2,$$

$$\left(\frac{1}{1-6t}\right)^5, |t| < \frac{1}{6}.$$

$$E(e^{yt}) = \left(\frac{1}{1-6t}\right)^8, |t| < \frac{1}{6}.$$

b) Gamma $\alpha = 8, \beta = 6.$

$$g(y) = \begin{cases} \frac{y^7 e^{-\frac{y}{6}}}{\Gamma(8)6^8}, & y > 0. \\ 0, & \text{otherwise.} \end{cases}$$

84b) $x_i \sim Posiison(\mu_i), i = 1, 2, ..., n$. $y = x_1 + x_2 + \cdots + x_n$.

$$E(e^{ty}) = E(e^{t\sum_{i=1}^{n} x_i}) = E(\prod_{i=1}^{n} e^{tx_i}) = \prod_{i=1}^{n} E(e^{tx_i}).$$

$$f(x_i) = \begin{cases} \frac{\mu_i^{x_i} e^{-\mu_i}}{x_i!}, & x_i = 0, 1, 2, ... \\ 0, & \text{otherwise.} \end{cases}$$

$$\prod_{i=1}^{n} E(e^{tx_i}) = \prod_{i=1}^{n} e^{\mu_i(e^t-1)} = e^{\sum_{i=1}^{n} \mu_i(e^t-1)}$$

which is Poisson $(\mu_1 + \mu_2 + \cdots + \mu_n)$.

13.32 References

1. Feller, W. (1968), *An Introduction to Probability Theory and Its Applications, Volume 2,* John Wiley & Sons, New York.

Chapter 14

Mathematical Statistics II

Dr. Dahiya, Old Dominion University
Statistics 626, Spring 1997
Text used: Hogg, Robert V. and Allen T. Craig, *Introduction to Mathematical Statistics, 5-th edition,* Prentice Hall, Upper Saddle River, NJ, 1995

Chapters 6 through 11 of the text book will be covered. There will be 4 sets of homework worth 25%, a midterm worth 30%, and the final exam will be worth 45%. Office hours are from 2:00-3:00pm on Monday and Wednesday.

14.1 Background

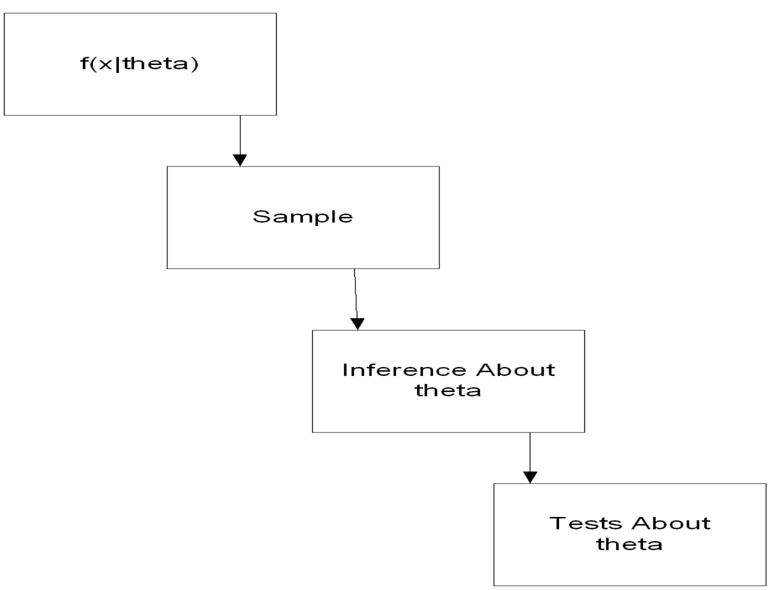

Figure 14.1: Selecting a statistical model.

Suppose x is a random variable. Assume x has the pdf $f(x|\theta), \theta \in \Omega$. The model to follow for this course is given in Figure 14.1. How do we select the model? Study the physical properties of different models.

- Shape.
- Symmetry.
- Skewness.
- Special properties of different distributions.

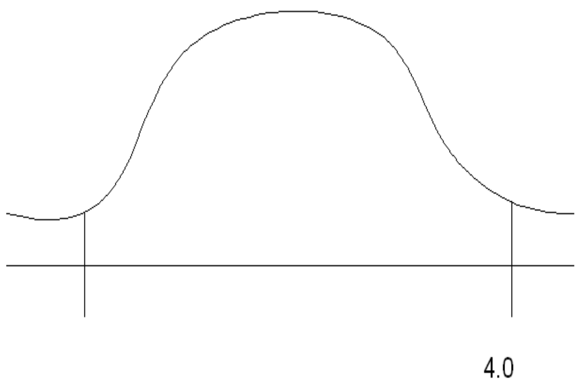

Figure 14.2: A truncated, normal distribution.

Example: Let the random variable x be the GPA of a selected student. By the Central Limit Theorem, x is normally distributed. Figure 14.2 shows a *truncated normal distribution,* because $-\infty$ and ∞ are not appropriate. So, our truncation is $[x|a < x < b]$. Then,

$$f^*(x|\theta)\,dx = \frac{f(x|\theta)\,dx}{P(a < x < b)} = \frac{f(x|\theta)\,dx}{F(b) - F(a)}.$$

Example: Let the random variable x be the height of a selected adult female student. This has a normal distribution. If x is the height of an ODU student, then it includes both males and females. Thus, it is a mixture of two normal distributions.

Exponential Distribution

$x \sim exp(\theta)$, if $f(x) = \frac{1}{\theta}e^{-x/\theta}, x > 0, \theta > 0$. Suppose that the random variable x is the life span of a certain animal. The life span cannot be exponential because $P(x > a + b|x > b) = P(x > a)$. This is called the *lack of memory property.*

```
-----(---)---------------(---)--------  time
        |                   |
        |                   |
        |                   |
        Death here         Same as death here
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Gamma Distribution

If $x_1, x_2, ..., x_k$ are iid $exp(\theta)$, then $y = \sum_{i=1}^{k} x_i \sim Gamma(k, \theta)$. If a part has an exponential distribution and you have k spare parts, then y is the time to failure of all k parts. $y \sim Gamma(k, \theta)$.

Relationship Between the Poisson and Exponential

Let x be the time in between two Poisson events. Then, $x \sim exp(\theta), \theta = \frac{1}{\lambda}$. Look at k Poisson events, then it is a Gamma distribution.

Poisson Distribution

Let x be the number of fires in Norfolk in a week. Recall that the binomial distribution approaches the Poisson distribution as $n \to \infty$ and $p \to 0$, such that $np = \lambda$. Let n be the number of houses in Norfolk. $p = P($ given house catches fire during a week$)$.

Uniform Distribution

If $x \sim U(0,1)$ then, $f(x)\,dx = 1\,dx, 0 < x < 1$. Let y be a continuous random variable with the density function $f(y|\theta)\,dy$. The distribution function is $F(y) = P(Y \leq y)$. What is the distribution of $x = F(y)$? $\frac{dx}{dy} = f(y|\theta) \Rightarrow dx = f(y|\theta)\,dy$. Therefore, x has a Uniform(0,1) distribution. Regardless of the distribution used, it will still be a uniform distribution. This relationship can be used to generate any continuous distribution if $x = F(y)$ can be inverted, $y = F^{-1}(x)$.

Example: Let $y \sim exp(\theta)$. Then, $F(y) = 1 - e^{-\frac{y}{\theta}}$, $x = F(y) \Rightarrow x = 1 - e^{-\frac{y}{\theta}} \Rightarrow y = -\theta \log(1-x)$ where x is uniform.

Importance of Means and Variances

Why are means and variances so important? Suppose there are two states. Look at the income of each state A and B. The distribution of state A is $f_x(x|\theta)$ and the distribution of state B is $f_y(y|\beta)$. What is $P(a < x < b)$ and $P(a < y < b)$? If the parameters are the same, then everything above is the same. Which means that the *means* are the same.

14.2 Estimation of Parameters

Suppose x has the pdf $f(x|\theta), \theta \in \Omega$. Take a random sample $x_1, x_2, ..., x_n$ and the random sample is iid with the same distribution as x. $\widehat{\theta} = u(x_1, x_2, ..., x_n)$ is completely specified by the random sample and is a point estimate of θ.

Desirable Properties of $\widehat{\theta}$

1. Let $\widetilde{\theta}$ be another estimator of θ. $P(-a < \widehat{\theta} - \theta < a) > P(-a < \widetilde{\theta} - \theta < a)$.

2. $\widehat{\theta} - \theta$ is called the *error in* $\widehat{\theta}$ for estimating θ. $E[\widehat{\theta} - \theta] = B(\theta)$ is called the *bias in* $\widehat{\theta}$. If $B(\theta) = 0$ then $\widehat{\theta}$ is unbiased for θ.

3. $Var(\widehat{\theta} - \theta) = Var(\widehat{\theta})$ should be as small as possible. Sometimes we look at the mean square error called $MS(E)$. $E(\widehat{\theta} - \theta)^2 = MS(E)$ of $\widehat{\theta}$. It should be as small as possible. The $MS(E)$ is a better comparison method.

$$MS(E) = E(\widehat{\theta} - \theta)^2 = E(\widehat{\theta} - \mu_\theta + \mu_\theta - \theta)^2 = E[(\widehat{\theta} - \mu_\theta)^2 + (\mu_\theta - \theta)^2 + 2(\mu_\theta - \theta)(\widehat{\theta} - \mu_\theta)] =$$

$$Var(\widehat{\theta}) + B(\theta)^2 + 0 = Var(\widehat{\theta}) + B(\theta)^2 = MSE(\widehat{\theta}).$$

Here, $\mu_\theta = E(\widehat{\theta}), \mu_\theta - \theta = E(\widehat{\theta}) - \theta = E(\widehat{\theta} - \theta) = B(\theta)$. If $\widehat{\theta}$ is unbiased, then $MSE(\widehat{\theta}) = Var(\widehat{\theta})$. Let T and T' be two different estimates of θ. If $P(\lambda_1 < T - \theta < \lambda_2) \geq P(\lambda_1 < T' - \theta < \lambda_2)$, then $E(T - \theta)^2 \leq E(T' - \theta)^2$ or $MSE(T) \leq MSE(T')$.

Without assuming any distribution, how do we estimate μ and σ^2?

Estimation of μ

Let $x_1, x_2, ..., x_n$ be a random sample. Suppose $\sum_{i=1}^{n} a_i = 1$. $\widetilde{\mu} = \sum a_i x_i$ is an unbiased estimator of μ because $E(\sum a_i x_i) = \sum a_i E(x_i) = \mu \sum a_i = \mu$. Look at $Var(\widetilde{\mu}) = Var(\sum a_i x_i) = \sum Var(a_i x_i)^2 = \sum a_i^2 Var(x_i) = \sigma^2 \sum a_i^2$. We wish to minimize $\sum a_i^2$ subject to $\sum a_i = 1$. It is minimized when $a_i = \frac{1}{n}$. $\widehat{\mu} = \sum \frac{x_i}{n} = \bar{x}$. In the class of linear functions of $x_1, x_2, ..., x_n$ $\bar{x}$ is the minimum variance unbiased estimator.

Estimation of σ^2

Let's take the second sample moment. $s^2 = \frac{1}{n-1} \sum (x_i - \bar{x})^2$. $E(s^2) = \sigma^2$ and $\widehat{\sigma} = s$. Consider the method of maximum likelihood estimator of θ.

Example: $x \sim Bernoulli(1, \theta)$. Take a random sample $x_1, x_2, ..., x_n$.

$$P(X_1 = x_1, X_2 = x_2, ..., X_n = x_n) = \prod \theta^{x_i}(1-\theta)^{1-x_i} = \theta^{\sum_{i=1}^{n} x_i}(1-\theta)^{n-\sum_{i=1}^{n} x_i} = L(\theta|x).$$

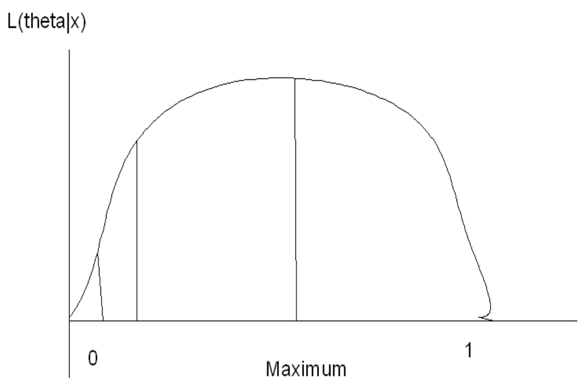

Figure 14.3: The maximum probability for θ.

Note that $f(x|\theta) = \theta^x (1-\theta)^{1-x}, x = 0, 1$. $\widehat{\theta}$ is the MLE of θ if $L(\widehat{\theta}|x) \geq L(\theta|x), \theta \in \Omega$. Maximizing $L(\theta|x)$ is the same as minimizing $\log L(\theta|x)$. See Figure 14.3. Then,

$$\log L(\theta|x) = \sum x_i \log \theta + (n - \sum x_i) \log(1-\theta).$$

$$\frac{d \log L}{d\theta} = \frac{\sum x_i}{\theta} - \frac{n - \sum x_i}{1-\theta} \Longrightarrow \theta = \frac{\sum x_i}{n}.$$

Thus, $\widehat{\theta} = \frac{\sum x_i}{n} = \bar{x}$ is the mle of θ. Let $y = \sum x_i \sim Binomial(n, \theta)$. $E(y) = n\theta$. $E\left(\frac{y}{n}\right) = \theta$ is unbiased. $Var(\widehat{\theta}) = \frac{\theta(1-\theta)}{n}$ In general, let x have the pdf $f(x|\theta)$ and let $x_1, x_2, ..., x_n$ be a random sample. $L(\theta|x) = \prod_{i=1}^{n} f(x_i|\theta)$.

Definition: $\widehat{\theta}$ is the *maximum likelihood estimator* of θ if $L(\widehat{\theta}|x) \geq L_{\theta \in \Omega}(\theta|x)$. Suppose we have the random sample (1, 0, 0, ..., 0, 1). See Figure 14.4. θ will be close to zero.

Example: $x \sim U(0, \theta)$,

$$f(x|\theta) = \begin{cases} \frac{1}{\theta}, & 0 < x_i < \theta. \\ 0, & \text{Otherwise.} \end{cases}$$

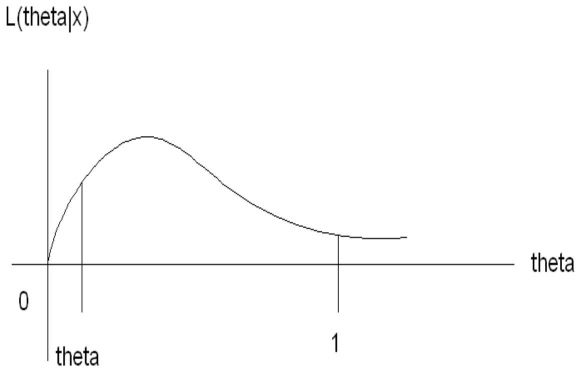

Figure 14.4: θ will be close to zero.

$$L(\theta|x) = \prod_{i=1}^{n} f(x_i|\theta) = \frac{1}{\theta^n}.$$

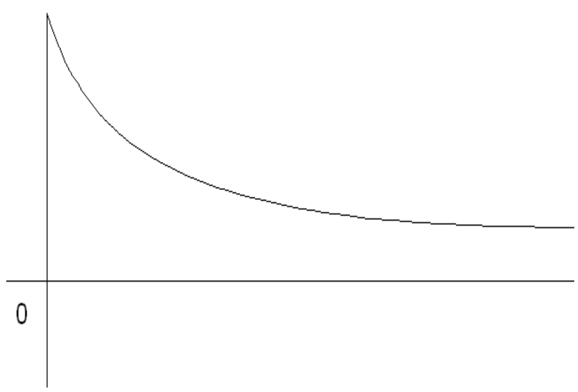

Figure 14.5: The uniform distribution example.

See Figure 14.5. Suppose that $x_{(n)} = \max(x_1, x_2, ..., x_n)$. Then the likelihood of θ is

$$L(\theta|x) = \begin{cases} \frac{1}{\theta^n}, & \text{if } \theta > x_{(n)}. \\ 0, & \text{otherwise.} \end{cases}$$

The correct graph can be found in Figure 14.6. The mle is $\widehat{\theta} = x_{(n)}$. $E(x) = \frac{\theta}{2} = \mu$ because $\widehat{\mu} = \bar{x}$ is unbiased. Then $\widetilde{\theta} = 2\bar{x}$ is unbiased for μ, but it is not acceptable because $f(x) = \frac{1}{\theta}$, $F(x) = \frac{x}{\theta}$. Since $2\bar{x}$ can be less than $x_{(n)}, \widehat{\theta}$ is not a desirable estimator.

Is $\widehat{\theta} = x_{(n)}$ biased or unbiased? We need the distribution of $x_{(n)}$. Look up the distribution of ordered statistics. The sample becomes $x_{(1)} \leq x_{(2)} \leq \cdots \leq x_{(n)}$. Then if $y = x_{(n)}$, the distribution of $x_{(n)}$ is

$$g(y) = nF(y)^{n-1} f(y) = n\frac{y^{n-1}}{\theta^{n-1}}\frac{1}{\theta} = \frac{ny^{n-1}}{\theta^n}.$$

Now find $E(x_{(n)})$.

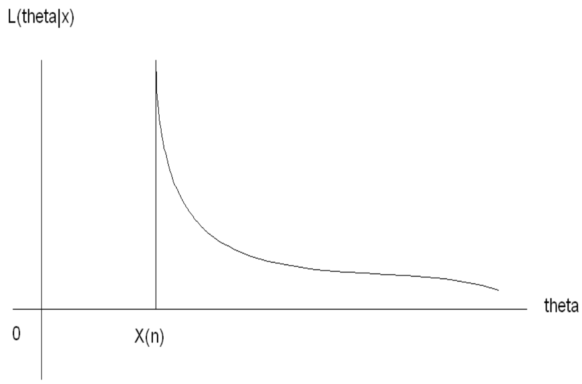

Figure 14.6: The $\max\{x_i\}$ distribution example.

$$E(x_{(n)}) = E(y) = \int_0^\theta \frac{y_n y^{n-1}}{\theta^n}\,dy = \frac{n}{\theta^n}\int_0^\theta y^n\,dy = \left.\frac{ny^{n+1}}{\theta^n(n+1)}\right|_0^\theta = \frac{n}{n+1}\theta = E(\widehat{\theta}).$$

Then, $E(\widehat{\theta}-\theta) = \frac{n}{n+1}\theta - \theta = -\frac{1}{n+1}\theta = B(\theta)$. Modify $\tilde{\theta}$ to be $\widehat{\theta}^* = \frac{n+1}{n}x_{(n)}$ and $E(\widehat{\theta}^*) = \frac{n+1}{n}E(x_{(n)}) = \frac{n+1}{n}\frac{n}{n+1}\theta = \theta$ and it is unbiased.

NOTE: When the support of the random variable involves a parameter, we need to examine the mle graphically.

Example: Let $x \sim N(\theta,1)$ and $f(x|\theta) = \frac{1}{\sqrt{2\pi}}e^{-\frac{(x-\theta)^2}{2}}$. Find the mle of θ $L(\theta|x) = \prod_{i=1}^n f(x_i|\theta) = \frac{1}{(2\pi)^{n/2}}e^{-\frac{\sum(x_i-\theta)^2}{2}}$. $\log L = c - \frac{\sum(x_i-\theta)^2}{2}$. Solve for $\frac{d\log L}{d\theta} = -(-)\frac{\sum(x_i-\theta)^2}{2} = 0 \Rightarrow \theta = \frac{\sum x_i}{n} \Rightarrow \widehat{\theta} = \bar{x}$ as the mle.

Example: Let $x \sim N(\theta_1,\theta_2)$ where $\theta_2 = Var(x)$. $f(x|\theta) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\theta_2}}e^{-\frac{(x-\theta_1)^2}{2\theta_2^2}}$.

$$L(\theta|x) = \prod_{i=1}^n f(x_i|\theta) = \frac{1}{(2\pi)^{n/2}\theta_2^{n/2}}e^{-\frac{\sum(x_i-\theta_1)^2}{2\theta_2}}$$

$$\log L = c - \frac{n}{2}\log\theta_2 - \frac{\sum(x_i-\theta_1)^2}{2\theta_2}$$

$$\frac{d\log L}{d\theta_1} = -(-)2\frac{\sum(x_i-\theta_1)}{2\theta_2} = 0 \Rightarrow \theta_1 = \bar{x}.$$

$$\frac{d\log L}{d\theta_2} = -\frac{n}{2\theta_2} - (-)\frac{\sum(x_i-\theta_1)^2}{2\theta_2^2} = 0 \Rightarrow \theta_2 = \frac{\sum(x_i-\theta_1)^2}{n}.$$

We cannot call it an estimator yet. Using the first and second equations,

$$\Rightarrow \widehat{\theta}_1 = \bar{x} \text{ is unbiased.}$$

$$\Rightarrow \widehat{\theta}_2 = \frac{1}{n}\sum(x_i-\bar{x})^2 \text{ is biased.}$$

$$E(\widehat{\theta}_2) = \frac{n-1}{n}E\left(\frac{n}{n-1}\sum(x_i-\bar{x})^2\right) = \frac{n-1}{n}\theta_2 = \theta_2 - \frac{1}{n}\theta_2 \text{ is biased.}$$

$$\tilde{\theta}_2 = \frac{n}{n-1}\widehat{\theta}_2 = \frac{1}{n-1}\sum(x_i - \bar{x})^2 = S^2 \text{ is unbiased.}$$

In the class of aS^2, the minimum $MS(E)$ estimator of θ_2 is given by $\frac{1}{n+1}\sum(x_i - \bar{x})^2$. That is, $E(\widehat{\theta}_2 - \theta_2)^2$ is the minimum if $\widehat{\theta}_2 = \frac{1}{n+1}\sum(x_i - \bar{x})^2$,

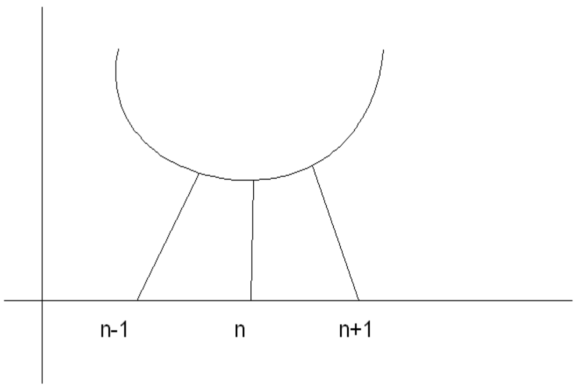

Figure 14.7: Choosing the MSE.

which is the difference from $\widehat{\theta}_2$ and $\tilde{\theta}_2$. Look at the $MS(E)$ of the mle's $E(\widehat{\theta}_2 - \theta_2)^2$ and $E(S^2 - \theta_2)^2 = MSE(S^2)$. See Figure 14.7. Choose the MS(E) of $\widehat{\theta}_2^2$ because of the division by $n+1$. Our choices were $a = \frac{1}{n+1}, a = \frac{1}{n}$, and $a = \frac{1}{n-1}$.

Example: $x \sim Gamma(\theta_1, \theta_2)$.

$$f(x|\theta) = \frac{e^{-x/\theta_1}x^{\theta_2 - 1}}{\Gamma(\theta_2)\theta_1^{\theta_2}}, \quad L(\theta|x) = \frac{e^{-\sum x_i/\theta_1}\prod_{i=1}^n x_i^{\theta_2 - 1}}{(\Gamma(\theta_2))^n \theta_1^{n\theta_2}}$$

Let $\sum x_i = T_1$, and $\prod x_i = T_2$. Then,

$$\log L = -\frac{T_1}{\theta_1} + (\theta_2 - 1)\log T_2 - n\theta_2 \log\theta_1 - n\log\Gamma(\theta_2),$$

$$\frac{d\log L}{d\theta_1} = \frac{T_1}{\theta_1^2} - \frac{n\theta_2}{\theta_1} = 0, \Rightarrow \theta_1 = \frac{T_1}{n\theta_2}.$$

But,

$$\frac{d\log L}{d\theta_2} = \log T_2 - n\log\theta_1 - \frac{n}{\Gamma(\theta_2)}\frac{d(\Gamma(\theta_2))}{d\theta_2} = 0.$$

We need to solve $\frac{d\log L}{d\theta_2}$ numerically.

$$\log T_2 - n\log\left(\frac{T_1}{n\theta_2}\right) - \frac{n}{\Gamma(\theta_2)}\frac{d(\Gamma(\theta_2))}{d\theta_2} = 0.$$

14.3 Consistent Estimator

Homework: Problems 6.1, 6.3, 6.5, 6.10, 6.18, 6.19, 6.34, 6.37, 6.38, 6.42, 6.43, 6.49, 6.54, 6.55, 6.56, 6.62, and 6.81 in the text book. Problems 6.38 and 6.42 are calculator answers. For problem 6.18, find the shortest confidence interval of σ based on a random sample of size n from $N(\mu, \sigma^2)$, where μ is unknown.

Definition: $\widehat{\theta}$ is *consistent* for θ if $\widehat{\theta}$ converges to θ. $\widehat{\theta} \to \theta$ as $n \to \infty$. Suppose $E(\widehat{\theta}) = \theta + B_n(\theta)$ where $B_n(\theta)$ is the bias. So, $B_n(\theta)$ must converge to zero as $n \to \infty$.

Sufficient Condition for Consistency: Let $B_n(\theta) = E(\widehat{\theta}) - \theta$ be the bias in $\widehat{\theta}$. Then $B_n(\theta) \to 0$ and $Var(\widehat{\theta}) \to 0$ implies consistency.

Proof:

$$P(|x - \mu| > \epsilon) < \frac{Var(x)}{\epsilon^2},$$

$$P(|\widehat{\theta} - \theta - B_n(\theta)| > \epsilon) < \frac{Var(x)}{\epsilon^2} \to 0,$$

$$\Rightarrow \widehat{\theta} - \theta - B_n(\theta) \to 0.$$

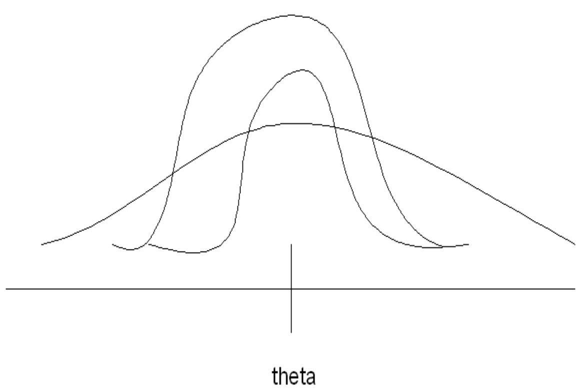

Figure 14.8: $x_n + y_n \to \theta$.

But, $B_n(\theta) \to 0 \Rightarrow \widehat{\theta} - \theta \to 0 \Rightarrow \widehat{\theta} \to \theta$. Suppose that $x_n \to \theta$ and $y_n \to 0$. Then, $x_n + y_n \to \theta + 0$. See Figure 14.8. Suppose that $\tilde{\theta}$ is not consistent.

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--------------(-|-)-------*-----------------
               theta
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$$P(\theta - \epsilon < \tilde{\theta} < \theta + \epsilon) \to 0,$$

$$\tilde{\theta} \to \theta^* = \theta + B_n(\theta).$$

Thus, do not use non-consistent estimators.

14.3.1 Estimating a Function of θ

Suppose $\phi = h(\theta)$ and $L(\theta|x) = \prod_{i=1}^{n} f(x_i|\theta)$. $L(\theta|x) = L(h^{-1}(\phi)|x) = L^*(\phi, x)$. Let $\widehat{\theta}$ be the mle of θ. Then, the mle is $\widehat{\phi} = h(\widehat{\theta})$ if it is a 1:1 function.

$$\frac{d\log L(h^{-1}(\phi)|x)}{d\phi} = \frac{d\log L(\theta|x)}{d\theta}\frac{d\theta}{d\phi} = 0 \Rightarrow \frac{d\log L}{d\theta} = 0.$$

Example: Let $x_1, x_2, ..., x_n$ be a random sample from $Poisson(\theta)$. $\phi = P(x=0) = e^{-\theta}$. We know $\widehat{\theta} = \bar{x}$, and $\widehat{\phi} = e^{-\bar{x}}$. $\widehat{\theta}$ is unbiased for θ since $E(\widehat{\theta}) = E(\bar{x}) = \theta$. Now, $E(\widehat{\phi}) = E(e^{-\bar{x}})$. Let $\bar{x} = \frac{\sum x_i}{n} = \frac{y}{n}$. Then, $y = \sum x_i \sim Poisson(n\theta)$. Then,

$$E(e^{-\bar{x}}) = E(e^{-y/n}) = \sum_{y=0}^{\infty} \frac{e^{-y/n}e^{-n\theta}(n\theta)^y}{y!} = e^{-n\theta(1-e^{-1/n})} = e^{-\theta}e^{-\frac{\theta}{2n}+\frac{\theta}{6n}} \to e^{-\theta} \text{ as } n \to \infty.$$

14.3.2 Use of Moment Estimators

Suppose $x \sim f(x|\theta)$. Suppose there is only a single parameter. $\mu = E(x) = \mu(\theta) = \int_{-\infty}^{\infty} x f(x|\theta)\,dx$ is called the *population mean*. The *sample mean* is $\bar{x} = \sum_{i=1}^{n} \frac{x_i}{n}$. The moment estimator of θ can be found by solving for $\mu(\theta) = \bar{x} \Rightarrow \tilde{\theta} = \mu(\bar{x})$. Is this going to be consistent? $\bar{x} = \frac{\sum x_i}{n} \to E(x) = \mu(\theta)$. Remember if $x_n \xrightarrow{P} a$, then the a continuous function $u(x_n) \xrightarrow{P} u(a)$ also. Then $\tilde{\theta} \xrightarrow{P} \theta$. Suppose we have two parameters $\underline{\theta} = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix}$. Compare the first two moments, $\mu_r' = E(x^r)$, and $m_r' = \frac{\sum x_i^r}{n}$. $\mu_1' = m_1'$ and $\mu_2' = m_2'$ implies $\mu = \bar{x}$ and $\sigma^2 = S^2 = \frac{1}{n}\sum(x_i - \bar{x})^2$. Solve $\bar{x} = \mu_1(\theta_1, \theta_2)$ and $S^2 = \mu_2(\theta_1, \theta_2)$.

Example: $x \sim Gamma(\theta_1, \theta_2)$.

$$f(x|\theta) = \frac{e^{-x/\theta_1}x^{\theta_2-1}}{\theta_1^{\theta_2}\Gamma(\theta_2)}, \;\; \mu = E(x) = \theta_1\theta_2, \;\; \sigma^2 = Var(x) = \theta_1\theta_2^2.$$

Solving $\theta_1\theta_2 = \bar{x}$ and $\theta_1\theta_2^2 = S^2$ implies $\widehat{\theta}_2 = \frac{S^2}{\bar{x}}$ and $\widehat{\theta}_1 = \frac{\bar{x}^2}{S^2}$. Moment estimators, in general, are consistent. $m_r' = \frac{\sum x_i^r}{n} = \frac{\sum y_i}{n}$ where $y_i = x_i^r$. Then, $y_i \xrightarrow{P} E(y_i) = E(x_i^r) = \mu_r'$. Consider the two functions $\tilde{\theta}_1 = u_1(m_1', m_2')$ and $\tilde{\theta}_2 = u_2(m_1', m_2')$. Then, $u_1(m_1', m_2') \xrightarrow{P} u_1(\mu_1', \mu_2') \Rightarrow \tilde{\theta}_1 \xrightarrow{P} \theta_1$ and $\tilde{\theta}_2 \xrightarrow{P} \theta_2$.

14.4 Homework and Answers

6.1 a.

$$f(x,\theta) = \frac{\theta^x e^{-\theta}}{x!}, x = 0, 1, 2...$$

$$f(x_i|\theta) = \begin{cases} \frac{\theta^{x_i}e^{-\theta}}{x_i!}, & x = 0, 1, 2...; 0 \le \theta < \infty. \\ 0, & \text{otherwise.} \end{cases}$$

$$\prod_{i=1}^{n} f(x_i|\theta) = \prod_{i=1}^{n} \frac{\theta^{x_i}e^{-\theta}}{x_i!} = \frac{\theta^{\sum x_i}e^{-n\theta}}{\prod x_i!} = L(\theta|\underline{x}).$$

$$\log L = \sum_{i=1}^{n} x_i \log\theta - n\theta - \log\prod_{i=1}^{n} x_i!,$$

$$\frac{d\log L}{d\theta} = \frac{1}{\theta}\sum_{i=1}^{n} x_i - n = 0 \Rightarrow \sum_{i=1}^{n} x_i - n\theta = 0,\ \ \sum_{i=1}^{n} x_i = n\theta,\ \ \frac{1}{n}\sum_{i=1}^{n} x_i = \widehat{\theta}.$$

b.

$$f(x,\theta) = \theta x^{\theta-1}, 0 < x < 1; 0 < \theta < \infty.$$

$$f(\theta|x_i) = \begin{cases} \theta x_i^{\theta-1}, & 0 < x < 1; 0 < \theta < \infty. \\ 0, & \text{otherwise.} \end{cases}$$

$$\prod_{i=1}^{n} \theta x_i^{\theta-1} = \theta^n \prod_{i=1}^{n} x_i^{\theta-1} = L(\theta|\underline{x}).$$

$$\log L = n\log\theta + (\theta-1)\log\prod_{i=1}^{n} x_i,$$

$$\frac{d\log L}{d\theta} = \frac{n}{\theta} + \log\prod_{i=1}^{n} x_i = 0 \Rightarrow n + \theta\log\prod_{i=1}^{n} x_i = 0,\ \ \theta\log\prod_{i=1}^{n} x_i = -n,\ \ \widehat{\theta} = \frac{-n}{\log\prod_{i=1}^{n} x_i}.$$

c.

$$f(\theta|x_i) = \begin{cases} \frac{e^{-x_i/\theta}}{\theta}, & 0 < x < \infty; 0 < \theta < \infty. \\ 0, & \text{otherwise.} \end{cases}$$

$$\prod_{i=1}^{n} f(\theta|x_i) = \prod_{i=1}^{n} \frac{e^{-x_i/\theta}}{\theta} = \frac{e^{-1/\theta\sum_{i=1}^{n} x_i}}{\theta^n} = L(\theta|x_i).$$

$$\log L = -\frac{1}{\theta}\sum_{i=1}^{n} x_i - n\log\theta,$$

$$\frac{d\log L}{d\theta} = \frac{1}{\theta^2}\sum_{i=1}^{n} x_i - \frac{n}{\theta} = 0,\ \ \sum_{i=1}^{n} x_i - n\theta = 0,\ \ -n\theta = -\sum_{i=1}^{n} x_i,\ \ \widehat{\theta} = \frac{1}{n}\sum_{i=1}^{n} x_i.$$

d. $L = e^{-\sum|x_i-\theta|}$. Minimize $h(\theta) = \sum|x_i - \theta|$.

$$\frac{d|x-\theta|}{d\theta} = \begin{cases} 1, & \text{if } x < \theta. \\ 0, & \text{if } x = \theta. \\ -1, & \text{if } x > \theta. \end{cases}$$

$x_{(1)} < x_{(2)} < \cdots < x_{(k)} < \theta < x_{(k+1)} < \cdots < x_{(n)}$. $\frac{dh}{d\theta} = k - (n-k) = 0 \Rightarrow k = \frac{n}{2}$.
If n is even, $k = \frac{n}{2}$ is an integer. For $n = 2m, k = m$, any θ in $(x_{(m)}, x_{(m+1)})$ is the mle. If n is odd, then k is not an integer. There are an equal number of $x's$ above and below θ. $n = 2m+1, \widehat{\theta} = x_{(m+1)}$ is the mle.

e. $L = e^{n\theta - \sum x_{(i)}}, \theta < x_{(1)} < \cdots < x_{(n)}$. Note that $L(\theta)$ increases in θ. So, $\widehat{\theta} = x_{(1)}$.

6.3

$$L(\theta|\underline{x}) = \begin{cases} 1, & x_{(n)} - \frac{1}{2} < \theta < x_{(1)} + \frac{1}{2}. \\ 0, & \text{otherwise.} \end{cases}$$

$t_1 = x_{(n)} - \frac{1}{2}$ and $t_2 = x_{(1)} + \frac{1}{2}$. The mle is not unique. Any average will be between t_1 and t_2. $\frac{4y_1+2y_n+1}{6}, y_1 = x_{(1)}, y_n = x_{(n)} = \frac{4t_2+2t_1}{6}$, and $\frac{y_1+y_n}{2} = \frac{t_1+t_2}{2}$.

6.5

$$F(x,\theta_1,\theta_2) = \begin{cases} 1-\left(\frac{\theta_1}{x}\right)^{\theta_2}, & \theta_1 \le x; \theta_1,\theta_2 > 0. \\ 0, & \text{otherwise.} \end{cases}$$

$$f(x,\theta_1,\theta_2) = \frac{dF}{dx} = \frac{d[1-\frac{\theta_1^{\theta_2}}{x^{\theta_2}}]}{dx} = \frac{d[1-\theta_1^{\theta_2}x^{-\theta_2}]}{dx} = -\theta_1^{\theta_2}x^{-\theta_2-1}(-\theta_2) = \theta_2\theta_1^{\theta_2}x^{-\theta_2-1}.$$

6.10

$$E(\widehat{\theta}) = E\left[\frac{\frac{x}{n}-\frac{x^2}{n^2}}{n}\right] = \frac{\frac{E(x)}{n}-\frac{E(x^2)}{n^2}}{n},$$

$$E(x) = np,\ \ Var(x) = E(x^2)-E(x)^2 = np(1-p) \Rightarrow E(x^2) = np(1-p)+n^2p^2.$$

Then,

$$E(\widehat{\theta}) = \frac{1}{n}\left[\frac{np}{n}-\frac{p(1-p)}{n}-p^2\right] = \frac{p}{n}\left[1-\frac{(1-p)}{n}-p\right] = \frac{p}{n}\left[\frac{n-1+p-np}{n}\right] =$$

$$\frac{p}{n}\left[\frac{n(1-p)-1+p}{n}\right] = \frac{p}{n}\left[\frac{n(1-p)-(1-p)}{n}\right] = \frac{p(1-p)(n-1)}{n^2}$$

which does not equal θ. Therefore, $\widehat{\theta}$ is biased. Multiply by $c=\frac{n}{n-1}$ to make the estimator unbiased.

6.18 a. We are given that $n=9, \alpha=0.05$ and that σ is known. To find the confidence interval,

$$0.05 = P\left(-z_{0.025} < \frac{(\bar{x}-\mu)\sqrt{9}}{\sigma} < z_{0.025}\right) = P\left(-1.96 < \frac{(\bar{x}-\mu)\sqrt{9}}{\sigma} < 1.96\right) =$$

$$P\left(-\frac{1.96\sigma}{3} < \bar{x}-\mu < \frac{1.96\sigma}{3}\right) = P\left(-\frac{1.96\sigma}{3}-\bar{x} < -\mu < \frac{1.96\sigma}{3}-\bar{x}\right) =$$

$$P\left(\bar{x}-\frac{1.96\sigma}{3} < \mu < \bar{x}+\frac{1.96\sigma}{3}\right),\ \ \left(\bar{x}-\frac{1.96\sigma}{3}, \bar{x}+\frac{1.96\sigma}{3}\right).$$

The length is 1.63σ.

b.

$$s^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i-\bar{x})^2,$$

The length is $1.63s$. We know that

$$y = \frac{ns^2}{\sigma^2} \sim \chi^2(n-1),\ \ s = \frac{\sigma}{\sqrt{n}}\sqrt{y}.$$

$$E(s) = \frac{\sigma}{\sqrt{n}}E(\sqrt{y}) = \frac{\sigma}{\sqrt{n}}\int_0^\infty \frac{\sqrt{y}e^{-y/2}y^{r/2-1}}{2^{r/2}\Gamma(r/2)}\,dy, r=n-1$$

$$\frac{\sigma}{\sqrt{n}}\frac{2^{(r+1)/2}\Gamma[(r+1)/2]}{2^{r/2}\Gamma(r/2)} = \sqrt{\frac{2}{n}}\sigma\frac{\Gamma(n/2)}{\Gamma[(n-1)/2]}.$$

6.19 $\bar{x} - x_{n+1} \sim N[0, \sigma^2(1/n+1)]$.

$$Var(\bar{x} - x_{n+1}) = \frac{n+1}{n}\sigma^2, \;\; \frac{ns^2}{\sigma^2} \sim \chi^2(n-1),$$

$$\frac{\frac{\bar{x}-x_{n+1}}{\sigma\sqrt{\frac{n+1}{n}}}}{\sqrt{\frac{ns^2}{\sigma^2(n-1)}}} = \frac{N(0,1)}{\sqrt{\chi^2(r)/r}} \sim t(r) = \sqrt{\frac{n-1}{n+1}}\frac{(\bar{x}-x_{n+1})}{s} \sim t(r).$$

Then, $c = \sqrt{\frac{n-1}{n+1}}$.

6.37 a.

$$s_1^2 = \sum_{i=1}^{n} \frac{(x_i - \bar{x})^2}{n}, \;\; s_2^2 = \sum_{i=1}^{m} \frac{(y_i - \bar{y})^2}{m}, \;\; F = \frac{\frac{ms_2^2}{\sigma_2^2}}{\frac{ns_1^2}{\sigma_1^2}}$$

has an F distribution with $m-1$ degrees of freedom in the numerator and $n-1$ degrees of freedom in the denominator.

b. If $P(F < b) = 0.975$ find a such that $P(F < a) = 0.025$. $P(a < F < b) = P(F < b) - P(F < a) = 0.975 - 0.025$. Without knowing n and m these values cannot be looked up. Professor's response: At least derive $1 - \alpha = P\left(a < \frac{\sigma_1^2}{\sigma_2^2} < b\right)$.

c.

$$P\left(\frac{a(m-1)}{(n-1)} < \frac{\frac{ms_2^2}{\sigma_2^2}}{\frac{ns_1^2}{\sigma_1^2}} < \frac{b(m-1)}{(n-1)}\right) = P\left(\frac{a(m-1)}{(n-1)(ms_2^2)} < \frac{\frac{1}{\sigma_2^2}}{\frac{ns_1^2}{\sigma_1^2}} < \frac{b(m-1)}{(n-1)(ms_2^2)}\right) =$$

$$P\left(\frac{a(m-1)(ns_1^2)}{(n-1)(ms_2^2)} < \frac{\frac{1}{\sigma_2^2}}{\frac{1}{\sigma_1^2}} < \frac{b(m-1)(ns_1^2)}{(n-1)(ms_2^2)}\right) = P\left(\frac{a(m-1)(ns_1^2)}{(n-1)(ms_2^2)} < \frac{\sigma_1^2}{\sigma_2^2} < \frac{b(m-1)(ns_1^2)}{(n-1)(ms_2^2)}\right) = 0.95.$$

6.38 $H_0 : \theta = 1$ versus $H_1 : \theta = 2$. The statistical power is given by

$$P(\text{Reject } H_0|H_1 \text{ true}) = P\left(\frac{3}{4} \le x_1x_2|\theta = 2\right),$$

$$f(x_1, x_2) = \begin{cases} 4x_1x_2, & 0 < x_1 < 1; 0 < x_2 < 1. \\ 0, & \text{otherwise.} \end{cases}$$

$$P\left(\frac{3}{4x_2} \le x_1 \middle| \theta = 2\right) = \int_{3/4}^{1}\int_{3/(4x_2)}^{1} 4x_1x_2\,dx_1\,dx_2 = \int_{3/4}^{1} 2x_1^2x_2\Big|_{3/(4x_2)}^{1} dx_2 = \int_{3/4}^{1} -\frac{2(9)}{16x_2^2}x_2 + 2x_2\,dx_2 =$$

$$\int_{3/4}^{1} 2x_2 - \frac{9}{8x_2}\,dx_2 = x_2^2 - \frac{9}{8}\ln x_2\Big|_{3/4}^{1} = 1 - 0 - \left[\frac{9}{16} - \frac{9}{8}\ln\frac{3}{4}\right] = \frac{7}{16} + \frac{9}{8}\ln\frac{3}{4}.$$

6.42 $x \sim N(\theta, 5000^2)$. $H_0 : \theta = 30000$, versus $H_1 : \theta > 30000$. $K(30000) = 0.01$ and $K(35000) = 0.98$. Reject H_0 when $\bar{x} \ge c$. Find n and c. $P(\text{Reject } H_0|\theta > 30000) = P(\bar{x} \ge c|\theta > 30000)$. $P\left(z \ge \frac{(c-30000)\sqrt{n}}{5000}\right) = 0.01$. and $P\left(z \ge \frac{(c-35000)\sqrt{n}}{5000}\right) = 0.98$. Solve the following two equations simultaneously. $\frac{(c-30000)\sqrt{n}}{5000} = 2.326$, $\frac{(c-35000)\sqrt{n}}{5000} = -2.05$. $(c-30000)\sqrt{n} = 2.326(5000)$, $c - 30000 = \frac{11630}{\sqrt{n}}$, $c = 30000 + \frac{11630}{\sqrt{n}}$. Substitute into the other equation to get $\frac{\left[30000+\frac{11630}{\sqrt{n}}-35000\right]\sqrt{n}}{5000} = -2.05$, $\left(\frac{11630}{\sqrt{n}} - 5000\right)\sqrt{n} = -10250$, $11630 - 5000\sqrt{n} = -10250$, $\sqrt{n} = 4.376 \Rightarrow n = 19.149$, Use $n = 20$. Back solve for c. $\frac{(c-30000)4.376}{5000} = 2.326$, $c - 30000 = 2657.68$, $c = 32657.68$.

6.43 $H_0 : \theta = \frac{1}{2}$ versus $H_1 : \theta < \frac{1}{2}$. $x \sim Poisson(\theta)$. $n = 12$. Reject H_0 if $y \leq 2$. $P(\text{Reject} H_0 | H_1 \text{ true}) = P\left(y \leq 2 | \theta < \frac{1}{2}\right) = P\left(\sum_{i=1}^{12} x_i \leq 2 | \theta < \frac{1}{2}\right) = P\left(12\bar{x} \leq 2 | \theta < \frac{1}{2}\right) = K(\theta)$. Using Table 1 in the back of the text book gives the following values for $K(\theta)$.

$$K\left(\frac{1}{2}\right) : 12\left(\frac{1}{2}\right) = 6; x = 2 \Rightarrow K(\theta) = 0.62.$$

$$K\left(\frac{1}{3}\right) : 12\left(\frac{1}{3}\right) = 4; x = 2 \Rightarrow K(\theta) = 0.238.$$

$$K\left(\frac{1}{4}\right) : 12\left(\frac{1}{4}\right) = 3; x = 2 \Rightarrow K(\theta) = 0.423.$$

$$K\left(\frac{1}{6}\right) : 12\left(\frac{1}{6}\right) = 2; x = 2 \Rightarrow K(\theta) = 0.677.$$

$$K\left(\frac{1}{12}\right) : 12\left(\frac{1}{12}\right) = 1; x = 2 \Rightarrow K(\theta) = 0.92.$$

$$\alpha = P(\text{Reject } H_0 | H_0 \text{ true}) = P\left(y \leq 2 | \theta = \frac{1}{2}\right) = P\left(6\bar{x} \leq 2 | \theta = \frac{1}{2}\right) = 0.062.$$

For the graph, simply plot θ on the x-axis and the power on the y-axis.

6.49 In this problem, we are given $p = 0.14, y = 104$, and $n = 590$.

a. $H_0 : p = 0.14$ versus $H_1 : p > 0.14$.

b. $\alpha = \text{P(Reject } H_0 | H_0 \text{ true)} = P(y \geq c | p = 0.14) = 0.01$.

$$P\left(\frac{y - np}{\sqrt{npq}} \geq \frac{c - np}{\sqrt{npq}}\right) = 0.01$$

$$P\left(z \geq \frac{c - 82.6}{8.428}\right) = 0.01 \Rightarrow \frac{c - 82.6}{8.428} = 2.326 \Rightarrow c = 102.20$$

c.

$$P\left(z \geq \frac{104 - 82.6}{8.428}\right) = 1 - \Phi(2.48)$$

$1 - 0.993 = 0.007$ which is the exact p-value

$y = 104$ is significant enough to reject the null hypothesis H_0. The proportion of drivers wearing seat belts after the advertising campaign has increased.

6.54 We are given $x \sim N(3, 4)$ and asked to calculate some probabilities.

$$P_{10} = P(x \leq 0) = 0.067.$$

$$P_{20} = P(0 < x \leq 1) = P(x \leq 1) - P(x < 0) = 0.159 - 0.067 = 0.092.$$

$$P_{30} = P(1 < x \leq 2) = P(x \leq 2) - P(x < 1) = 0.309 - 0.159 = 0.15.$$

$$P_{40} = P(2 < x \leq 3) = P(x \leq 3) - P(x < 2) = 0.50 - 0.309 = 0.191.$$

$$P_{50} = P(3 < x \leq 4) = P(x \leq 4) - P(x < 3) = 0.691 - 0.50 = 0.191.$$

$$P_{60} = P(4 < x \leq 5) = P(x \leq 5) - P(x < 4) = 0.841 - 0.691 = 0.15.$$

$$P_{70} = P(5 < x \leq 6) = P(x \leq 6) - P(x < 5) = 0.933 - 0.841 = 0.092.$$

$$P_{80} = P(6 < x < \infty) = P(x < \infty) - P(x < 6) = 1 - 0.933 = 0.067.$$

$$n = \sum_{i=1}^{8} n_i = 60 + 96 + 140 + 210 + 172 + 160 + 88 + 74 = 1000.$$

$$Q_7 = \sum_{i=1}^{8} \frac{(n_i - np_i)^2}{np_i} = \frac{(60-67)^2}{67} + \frac{(96-92)^2}{92} + \frac{(140-150)^2}{150} +$$

$$\frac{(210-191)^2}{191} + \frac{(172-191)^2}{191} + \frac{(160-150)^2}{150} + \frac{(88-92)^2}{92} + \frac{(74-67)^2}{67} = 6.924.$$

The cut-off value is $\chi^2_{0.05}(7) = 14.07$. Since $6.924 < 14.07$, we fail to reject H_0.

6.55 $\chi^2(5) = 12.83$. $p_1 = p_2 = \cdots = p_6 = \frac{1}{6}$ implies an unbiased die.

$$Q_5 = \frac{(b-20)^2}{20} + 0 + \cdots + \frac{(40-b-20)^2}{20} = \frac{b^2 - 40b + 400}{20} + \frac{400 - 40b + b^2}{20},$$

$\frac{b^2-40b+400}{10} = 12.83$. The roots are $\frac{4 \pm \sqrt{16 - 4(\frac{1}{10})(27.17)}}{2(\frac{1}{10})}$, $b = 31.33$ and $b = 8.673$. Choose $b \geq 32$ and $b \leq 8$.

6.56 $p_1 = \frac{9}{16}, p_2 = \frac{3}{16}, p_3 = \frac{3}{16}$, and $p_4 = \frac{1}{16}$ and $n = 160$. $Q_3 = \frac{(86-90)^2}{90} + \frac{(35-30)^2}{30} + \frac{(26-30)^2}{30} + \frac{(13-10)^2}{10} = 2.44$. The cut-off value is $\chi^2_{0.01}(3) = 11.3$. Since $2.44 < 11.3$, fail to reject H_0. The data is consistent with Mendelian Theory.

6.62 a. $f(x) = \frac{2x}{\theta^2}$.

$$F(x) = \int_0^x \frac{2w}{\theta^2} dw = \left. \frac{w^2}{\theta^2} \right|_0^x = \frac{x^2}{\theta^2}.$$

$$f(y_n) = \frac{n!}{(n-1)!} \frac{2y_n}{\theta^2} \left(\frac{y_n^2}{\theta^2} \right)^{n-1} = \frac{2ny_n}{\theta^2} \left(\frac{y_n^{2n-2}}{\theta^{2n-2}} \right) = \frac{2ny_n^{2n-1}}{\theta^{2n}}.$$

$$P\left(c < \frac{y_n}{\theta} < 1 \right) = P(c\theta < y_n < \theta) = \int_{c\theta}^{\theta} \frac{2ny_n^{2n-1}}{\theta^{2n}} dy_n = \left. \frac{y_n^{2n}}{\theta^{2n}} \right|_{c\theta}^{\theta} = \frac{\theta^{2n}}{\theta^{2n}} - \frac{c^{2n}\theta^{2n}}{\theta^{2n}} = 1 - c^{2n}.$$

b. Begin by using $1 - c^{2n} = 1 - c^{10} = 0.99$ and find the confidence interval.

14.5 Interval Estimation

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--------------(-|-)------------------------
               theta
```

Suppose that $\widehat{\theta}$ is an estimator of θ. $\widehat{\theta}$ is a *point estimator.* We need to form a statistic $u(\widehat{\theta}, \theta)$ whose distribution does not depend on θ. **General method:** The mle is the solution of

$$\frac{d \log L}{d\theta} = 0 \Rightarrow \frac{d \log f(x_i|\theta)}{d\theta} = 0 \Rightarrow E\left[\frac{d \log f(x_i|\theta)}{d\theta} \right] = 0, \quad I(\theta) = -E\left[\frac{d^2 \log L}{d\theta^2} \right], \quad \frac{\frac{d \log L}{d\theta}}{\sqrt{I(\theta)}} \to N(0,1).$$

Example: $x \sim N(\theta, \sigma^2)$ where σ is known. $\widehat{\theta} = \bar{x} \sim N(\theta, \sigma^2/n)$ does depend on θ. But, $z = \frac{\sqrt{n}(\widehat{\theta} - \theta)}{\sigma} \sim N(0,1)$. Then,

$$1 - \alpha = P\left(-z_{\alpha/2} < \frac{\sqrt{n}(\widehat{\theta} - \theta)}{\sigma} < z_{\alpha/2} \right) = P\left(\widehat{\theta} - \frac{\sigma}{\sqrt{n}} z_{\alpha/2} < \theta < \widehat{\theta} + \frac{\sigma}{\sqrt{n}} z_{\alpha/2} \right).$$

Then, we say the $(1-\alpha)100\%$ confidence interval is $\left(\widehat{\theta} - \frac{\sigma}{\sqrt{n}} z_{\alpha/2}, \widehat{\theta} + \frac{\sigma}{\sqrt{n}} z_{\alpha/2} \right)$

```
---------(--(---(-|-)---)--)-------------------
                theta
```

We do not want a very small α because the confidence interval will be wide. The length of the confidence interval is $2z_{\alpha/2}\frac{\sigma}{\sqrt{n}}$. This is because $2z_{\alpha/2} \leq (z_{\alpha_1}+z_{\alpha_2})$ where $\alpha_1+\alpha_2=\alpha$ and the distribution is symmetric. We must know σ to determine the sample size.

Example: $x \sim Binomial(n,p)$. $\widehat{p}=\frac{x}{n}$. For large n, $\frac{\widehat{p}-p}{\sqrt{\frac{pq}{n}}} \to N(0,1)$.

$$1-\alpha = P\left(-z_{\alpha/2} < \frac{\widehat{p}-p}{\sqrt{\frac{pq}{n}}} < z_{\alpha/2}\right) = P\left(\frac{n(\widehat{p}-p)^2}{p(1-p)} \leq z^2_{\alpha/2}\right)$$

$$\Rightarrow u(p) = p^2\left(1+\frac{z^2_{\alpha/2}}{n}\right) - \left(2\widehat{p}+\frac{z^2_{\alpha/2}}{n}\right)p + \widehat{p}^2 \leq 0.$$

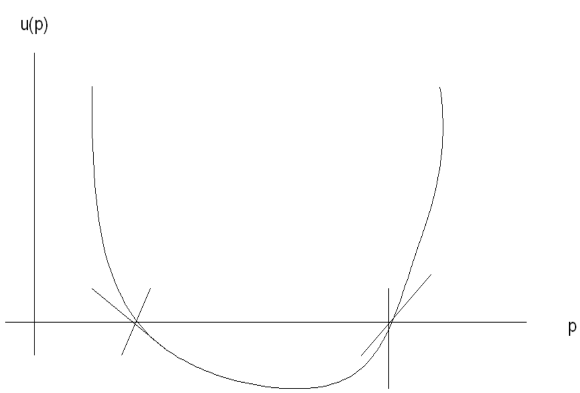

Figure 14.9: Solve for two values of p.

See Figure 14.9.

$$\widehat{p}+\frac{z^2_{\alpha/2}}{2n} \pm z_{\alpha/2}\sqrt{\left(\frac{\widehat{p}\widehat{q}}{n}+\frac{z^2_{\alpha/2}}{4n^2}\right)} \Big/ \left(1+\frac{z^2_{\alpha/2}}{n}\right)$$

$$\frac{\widehat{p}-p}{\sqrt{\frac{\widehat{p}\widehat{q}}{n}}} \sim N(0,1).$$

Now,

$$1-\alpha = P\left(-z_{\alpha/2} < \frac{\widehat{p}-p}{\sqrt{\frac{\widehat{p}\widehat{q}}{n}}} < z_{\alpha/2}\right) = P\left(\widehat{p}-z_{\alpha/2}\sqrt{\frac{\widehat{p}\widehat{q}}{n}} < p < \widehat{p}+z_{\alpha/2}\sqrt{\frac{\widehat{p}\widehat{q}}{n}}\right).$$

$\widehat{p} \pm z_{\alpha/2}\sqrt{\frac{\widehat{p}\widehat{q}}{n}}$ is called a $(-\alpha)00\%$ confidence interval of p for large n. The first expression is better because $\frac{\widehat{p}-p}{\sqrt{\frac{\widehat{p}\widehat{q}}{n}}} = \frac{\widehat{p}-p}{\sqrt{\frac{pq}{n}}}\frac{\sqrt{\frac{pq}{n}}}{\sqrt{\frac{\widehat{p}\widehat{q}}{n}}}$ even though it is not symmetric. Here is some more information on the confidence interval for the binomial p. The *error term* is $z_{\alpha/2}\sqrt{\frac{\widehat{p}\widehat{q}}{n}}$. Assume that $\alpha = 0.05, z_{0.025} = 1.96$, and $\epsilon = 0.03$. Then, $1.96\sqrt{\frac{\widehat{p}\widehat{q}}{n}} = 0.03 \Rightarrow n = \frac{(1.96)^2\widehat{p}\widehat{q}}{(0.03)^2}$

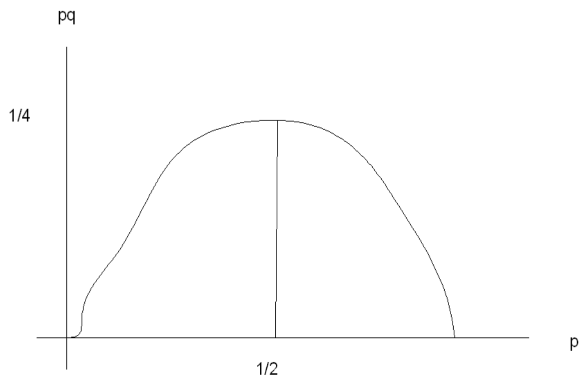

Figure 14.10: The maximum pq can be is $pq = \frac{1}{4}$.

See Figure 14.10. The maximum $p \times q$ can be is $p \times q = \frac{1}{4}$. $\Rightarrow n \leq \frac{(1.96)^2}{(0.03)^2}\frac{1}{4} \leq 1067$. Suppose that $x \sim N(\theta, \sigma^2)$ and σ is unknown. Find the confidence interval of θ. Before, we used $z = \frac{\sqrt{n}(\bar{x}-\theta)}{\sigma}$. But, σ is unknown. Let $S^2 = \frac{1}{n-1}\sum(x_i - \bar{x})^2$. Then,

$$T = \frac{\sqrt{n}(\bar{x}-\theta)}{S} = \frac{(\bar{x}-\theta)/(\sigma/\sqrt{n})\sigma}{\sigma\sqrt{\chi^2(n-1)/(n-1)}} = \frac{N(0,1)}{\sqrt{\frac{\chi^2(n-1)}{n-1}}} \sim t(n-1).$$

Then,

$$1-\alpha = P\left(-t_{\alpha/2}(r) < \frac{n(\bar{x}-\theta)}{S} < t_{\alpha/2}(r)\right) = P\left(\bar{x} - t_{\alpha/2}(r)\frac{S}{\sqrt{n}} < \theta < \bar{x} + t_{\alpha/2}(r)\frac{S}{\sqrt{n}}\right).$$

Note that $\frac{(n-1)S^2}{\sigma^2} \sim \chi^2(n-1)$ and that $S^2 = \frac{\sigma^2\chi^2(n-1)}{n-1}$. The $100\%(1-\alpha)$ confidence interval is then $\bar{x} \pm t_{\alpha/2}(r)\frac{S}{\sqrt{n}}$. Note that when σ was known, we had $\bar{x} \pm z_{\alpha/2}\frac{\sigma}{\sqrt{n}}$. To compare the two lengths, we need to find $2t_{\alpha/2}(r)\frac{E(S)}{\sqrt{n}}$. Note that $\frac{t(r)}{\sqrt{Var(t(r))}} \to N(0,1)$ as $r \to \infty$.

14.5.1 Comparing Two Means

Suppose that $x \sim N(\mu_x, \sigma_x^2)$ with a random sample of $x_1, x_2, ..., x_n$ and $y \sim N(\mu_y, \sigma_y^2)$ with a random sample of $y_1, y_2, ..., y_m$. Find the confidence interval of $\mu_x - \mu_y$. Assume that σ_x and σ_y are known. $\bar{x} - \bar{y}$ is an estimator of $\mu_x - \mu_y$. $\bar{x} - \bar{y} \sim N(\mu_x - \mu_y, \sigma_x^2/n + \sigma_y^2/m)$. Then,

$$\frac{\bar{x} - \bar{y} - (\mu_x - \mu_y)}{\sqrt{\frac{\sigma_x^2}{n} + \frac{\sigma_y^2}{m}}} \sim (0,1).$$

Based on that, the confidence interval is

$$\bar{x} - \bar{y} \pm z_{\alpha/2}\sqrt{\frac{\sigma_x^2}{n} + \frac{\sigma_y^2}{m}}$$

If σ_x and σ_y are unknown and n and m are small, then $\frac{(n-1)s_x^2}{\sigma_x^2} \sim \chi^2(n-1)$, and $\frac{(m-1)s_y^2}{\sigma_y^2} \sim \chi^2(m-1)$.

$$\frac{\bar{x}-\bar{y}-(\mu_x-\mu_y)}{\sqrt{\frac{S_x^2}{n}+\frac{S_y^2}{m}}} = \frac{[\bar{x}-\bar{y}-(\mu_x-\mu_y)]\Big/\sqrt{\frac{\sigma_x^2}{n}+\frac{\sigma_y^2}{m}}}{\sqrt{\frac{\chi^2(n-1)}{n-1}\frac{\sigma_x^2}{n}+\frac{\chi^2(m-1)}{m-1}\frac{\sigma_y^2}{m}}} \times \sqrt{\frac{\sigma_x^2}{n}+\frac{\sigma_y^2}{m}}.$$

There is no cancelation above. But if $\sigma_x = \sigma_y = \sigma$ and we use the pooled estimate of σ, then cancelation occurs. Note that,

$$\frac{\bar{x}-\bar{y}-(\mu_x-\mu_y)}{\sigma\sqrt{\frac{1}{n}+\frac{1}{m}}} \sim N(0,1).$$

But, using the pooled estimator, where $s_p = \frac{(n-1)s_x^2+(m-1)s_y^2}{n+m-2}$, we get $\frac{\bar{x}-\bar{y}-(\mu_x-\mu_y)}{s_p\sqrt{\frac{1}{n}+\frac{1}{m}}} \sim t(r)$, where the degrees of freedom r is $r = n+m-2$. That is the definition of the t distribution. To prove that it has a t distribution, if $x \sim N(0,1)$ and $y \sim \chi^2(r)$ and both x and y are independent random variables, then $\frac{x}{\sqrt{\frac{\chi^2(r)}{r}}} \sim t(r)$. Finally, the confidence interval is

$$\bar{x}-\bar{y} \pm t_{\alpha/2}(r)s_p\sqrt{\frac{1}{n}+\frac{1}{m}}.$$

Find the confidence interval of $\mu_x - a\mu_y$ where a is a known constant and $\sigma_x = \sigma_y = \sigma$.

$$\bar{x}-a\bar{y} \sim N\left(\mu_x - a\mu_y, \sigma^2\left[\frac{1}{n}+\frac{a^2}{m}\right]\right).$$

$$\frac{\bar{x}-a\bar{y}-(\mu_x-a\mu_y)}{\sigma\sqrt{\frac{1}{n}+\frac{a^2}{m}}} \sim N(0,1).$$

To get a confidence interval in a t distribution,

$$\frac{\bar{x}-a\bar{y}-(\mu_x-a\mu_y)}{s_p\sqrt{\frac{1}{n}+\frac{a^2}{m}}} \sim t(r).$$

Suppose that $\sigma_x \neq \sigma_y$, but $\frac{\sigma_x}{\sigma_y} = a$ is known. Next, find the confidence interval of $\mu_x - \mu_y$. Prove this for homework.

14.5.2 Confidence Intervals for Two Binomials

Suppose that $x \sim Binomial(n, p_1)$ and $y \sim Binomial(m, p_2)$. $\widehat{p}_1 = \frac{x}{n}$ and $\widehat{p}_2 = \frac{y}{m}$. Find the interval estimation of $p_1 - p_2$. Note that $E(\widehat{p}_1) = p_1$ and that $Var(\widehat{p}_1) = \frac{p_1 q_1}{n}$. Similar expressions hold for $\widehat{p}_2$. Assuming that n and m are large, then

$$\frac{\widehat{p}_1-\widehat{p}_2-(p_1-p_2)}{\sqrt{\frac{\widehat{p}_1\widehat{q}_1}{n}+\frac{\widehat{p}_2\widehat{q}_2}{m}}} \to N(0,1).$$

The $(1-\alpha)100\%$ confidence interval of $p_1 - p_2$ is

$$\widehat{p}_1 - \widehat{p}_2 \pm z_{\alpha/2}\sqrt{\frac{\widehat{p}_1\widehat{q}_1}{n} + \frac{\widehat{p}_2\widehat{q}_2}{m}}$$

14.5.3 Confidence Intervals of σ

Let the random variable x have the distribution $x \sim N(\mu, \sigma^2)$. Assume that μ is known and $x_1, x_2, ..., x_n$ is a random sample. The mle of σ^2 is $\widehat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^n (x_i - \mu)^2$. It is know that $\frac{n\widehat{\sigma}^2}{\sigma^2} = \frac{\sum_{i=1}^n (x_i-\mu)^2}{\sigma^2} = \sum_{i=1}^n z_i^2$ where $z_1, z_2, ..., z_n$ are iid $N(0,1)$. Thus, $\sum_{i=1}^n z_i^2 \sim \chi^2(n)$. Find the constants a and b such that

$$P(a < \chi^2(n) < b) = 1-\alpha = P\left(a < \frac{n\widehat{\sigma}^2}{\sigma^2} < b\right) = P\left(\frac{1}{b} < \frac{\sigma^2}{n\widehat{\sigma}^2} < \frac{1}{a}\right) = P\left(\frac{n\widehat{\sigma}^2}{b} < \sigma^2 < \frac{n\widehat{\sigma}^2}{a}\right).$$

The length of the confidence interval $\frac{n\widehat{\sigma}^2}{a} - \frac{n\widehat{\sigma}^2}{b} = \frac{n\widehat{\sigma}^2(b-a)}{ab}$ will not work. We want to minimize $\frac{(b-a)}{ab}$ subject to $G_n(b) - G_n(a) = 1-\alpha$. $G_n(x) = P(\chi^2(n) < x)$. The confidence interval for σ is

$$1-\alpha = P\left(\sqrt{\frac{n\widehat{\sigma}^2}{b}} < \sigma < \sqrt{\frac{n\widehat{\sigma}^2}{a}}\right).$$

Thus the length of the confidence interval is $\sqrt{n\widehat{\sigma}^2}\left(\frac{\sqrt{b}-\sqrt{a}}{\sqrt{ab}}\right)$. In other courses you will find $x \sim$ log normal if $y = \log x \sim N(\mu, \sigma^2)$. The same problem of finding the shortest confidence interval length arises. $P(a < y < b) = 1-\alpha = P\left(e^a < e^y < e^b\right) = P\left(e^a < x < e^b\right)$.
Now suppose that μ is unknown. The estimator for σ becomes

$$\widehat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^n (x_i - \bar{x})^2, \;\; S^2 = \frac{1}{n-1}\sum_{i=1}^n (x_i - \bar{x})^2.$$

Then, $\frac{(n-1)S^2}{\sigma^2} \sim \chi^2(n-1)$. $1-\alpha = P\left(\frac{(n-1)S^2}{b} < \sigma^2 < \frac{(n-1)S^2}{a}\right)$ where a and b are such that $G_r(b) - G_r(a) = 1-\alpha$ and $r = n-1$.

14.6 Testing Hypotheses

Example: Let the random variable x be the GPA of a student selected at random at ODU and $x \sim N(\theta, \sigma^2)$. Test the null hypothesis $H_0 : \theta = 2.5$ versus $H_1 : \theta > 2.5$. $\bar{x}$ is the estimator of θ. Assume that σ is known. If H_0 is true, then $\bar{x} \sim N(2.5, \sigma^2/n)$. If H_1 is true, then $\bar{x} \sim N(\theta_1, \sigma^2/n)$. When do we reject H_0? Reject for large values if $\bar{x} > c$.

	Reject H_0	Reject H_1
H_0 True	Type I Error	Correct
H_1 Ture	Correct	Type II Error

$H_1 : \theta = \theta_1 > 2.5$ for a specific θ_1. $P(\text{Reject } H_0|H_0) = \alpha$ which is the Type I error, which is equal to $P(\bar{x} > c|\theta = 2.5)$. The Type II error is $P(\text{Reject } H_1|H_1) = \beta = P(\bar{x} < c|\theta = \theta_1)$. For a fixed n, increasing c decreases α, but, β increases. Work with α first since β depends on θ_1. For fixed c and θ_1, both α and β

will decrease as n increases. α converges to zero since $\bar{x} \to 2.5$ The *power* is $1-\beta = P(\text{Reject } H_0|H_1)$. This is used for comparing two statistical tests. In the binomial example, p is the proportion of defectives. The hypotheses are $H_0 : p = p_0$ versus $H_1 : p > p_0$.

Example: Suppose $x \sim N(\theta, 1)$. $H_0 : \theta = 5$ versus $H_1 : \theta > 5$. Reject H_0 if $\bar{x} > c$. We need to find c for $\alpha = 0.05$. $0.05 = P(\text{Reject } H_0|H_0 \text{ true}) = P(\bar{x} > c|\theta = 5) = P\left(\frac{\bar{x}-5}{1/\sqrt{n}} > \frac{c-5}{1/\sqrt{n}}\middle|\theta = 5\right) = P(z > \sqrt{n}(c-5))$. Then, $\sqrt{n}(c-5) = 1.645 \Rightarrow c = \frac{1}{\sqrt{n}}(1.645) + 5$. The power is $P(\text{Reject } H_0|H_1 \text{ true}) = P\left(\bar{x} > \frac{1}{\sqrt{n}}(1.645) + 5\middle|\theta = \theta_1\right) P\left(\frac{\bar{x}-\theta_1}{1/\sqrt{n}} > (c-\theta_1)\sqrt{n}\middle|\theta = \theta_1\right) P\left(z > \left[5 + \frac{1}{\sqrt{n}}(1.645) - \theta_1\right]\sqrt{n}\right) = k(\theta_1) = P(z > 1.645 + (5-\theta_1)\sqrt{n}) \geq 0.05$. We need a specific n and θ_1 to find the power. Note that $k(\theta_1)$ increases as θ_1 increases and as $k(\theta_1)$ increases as n increases.

14.6.1 Testing About the Binomial p

Example: Suppose that $x \sim \textit{Binomial}(p)$. $n = 10$ and the hypotheses tests are $H_0 : p = \frac{1}{2}$ versus $H_1 : p > \frac{1}{2}$. We reject H_0 if $x \geq c$. To be more specific, let's reject H_0 if $x \geq 8$.

$$\alpha = P(\text{Reject } H_0|H_0 \text{ true}) = P\left(x \geq 8\middle|p = \frac{1}{2}\right) = \sum_{x=8}^{10} \binom{10}{x} \left(\frac{1}{2}\right)^{10} = 0.0547.$$

Since this is a discrete random variable, we can not find an exact $\alpha = 0.05$.

Binomial Randomized Test

We reject H_0 with a probability of 1 if $x \geq 9$. We reject H_0 with a probability of θ if $x = 8$. So, we carry out a randomized test if $x = 8$. $0.05 = P(\text{Reject } H_0|H_0 \text{ true}) = P(x \geq 9|H_0) + \theta P(x = 8) = 0.0107 + \theta(0.0547 - 0.0107) \Rightarrow \theta = 0.89$. Note that $x_1, x_2, ..., x_n$ are iid Bernoulli random variables. This is a random sample and has a Binomial distribution. Find the power $k(p) = P(\text{Reject } H_0|H_1 \text{ true}) = P\left(x \geq 8\middle|p = p_1 > \frac{1}{2}\right) = \sum_{x=8}^{10} \binom{10}{x} p_1^x q_1^{n-x}$ To find the power of the randomized test,

$$k(p_1) = P(\text{Reject } H_0|H_1 \text{ true}) = P(x \geq 9|H_1) + \theta P(x = 8|H_1) = \sum_{9}^{10} \binom{10}{x} p_1^x q_1^{n-x} + (0.89)\binom{10}{8} p_1^8 q_1^2.$$

The randomized binomial test has a smaller power than the original test. We can not compare the two unless α is the same in both tests.

14.6.2 Two-Sided Alternative Tests

Suppose that $x \sim N(\theta, \sigma^2)$ and σ is known. Consider the hypotheses $H_0 : \theta = \theta_0$ versus $H_1 : \theta \neq \theta_0$. Let $x_1, x_2, ..., x_n$ be a random sample. The test statistic is $z = \frac{\sqrt{n}(\bar{x}-\theta_0)}{\sigma} \sim N(0,1)$ under H_0. Reject H_0 for $|z| > z_{\alpha/2}$. $P(|z| > z_{\alpha/2}|H_0) = \alpha = 1 - P(-z_{\alpha/2} < z < z_{\alpha/2})$. The power of the test statistic is $k(\theta_1) = P(\text{Reject } H_0|H_1 \text{ true}) = P\left(\left|\frac{\sqrt{n}(\bar{x}-\theta_0)}{\sigma}\right| > z_{\alpha/2}\middle|H_1\right)$. $\beta(\theta_1) = 1 - k(\theta_1) = P\left(-z_{\alpha/2} < \frac{\sqrt{n}(\bar{x}-\theta_0)}{\sigma} < z_{\alpha/2}\middle|H_1\right) = P\left(\theta_0 - \frac{\sigma}{\sqrt{n}}z_{\alpha/2} < \bar{x} < \theta_0 + \frac{\sigma}{\sqrt{n}}z_{\alpha/2}\middle|H_1\right) = P\left((\theta_0-\theta_1)\frac{\sqrt{n}}{\sigma} - z_{\alpha/2} < \frac{(\bar{x}-\theta_1)\sqrt{n}}{\sigma} < (\theta_0-\theta_1)\frac{\sqrt{n}}{\sigma} + z_{\alpha/2}\right)$. $k(\theta_1) = P\left(z > (\theta_0-\theta_1)\frac{\sqrt{n}}{\sigma} + z_{\alpha/2}\right) + P\left(z < (\theta_0-\theta_1)\frac{\sqrt{n}}{\sigma} - z_{\alpha/2}\right)$

An Unbiased Test

If $k(\theta) \geq k(\theta_0)$, then the test is unbiased. The two sided test is related to the confidence intervals $\bar{x} \pm z_{\alpha/2}\frac{\sigma}{n}$. Accept H_0 if θ is in the confidence interval. Reject H_0 otherwise.

14.6.3 Testing About the Normal Mean When σ is Unknown

The estimator for σ^2 is $S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$. The possible hypotheses tests are $H_0 : \theta = \theta_0$ versus three possible alternative hypotheses: $H_1 : \theta > \theta_0$, $H_1 : \theta < \theta_0$, or $H_1 : \theta \neq \theta_0$. The test statistic has a t distribution. $T = \frac{(\bar{x}-\theta_0)\sqrt{n}}{S} \sim t(n-1)$ under H_0.

For H_1	Reject If
$\theta > \theta_0$	$T > t_\alpha(n-1)$
$\theta < \theta_0$	$T < -t_\alpha(n-1)$
$\theta \neq \theta_0$	$\lvert T\rvert > t_{\alpha/2}(n-1)$

To find the power for the hypotheses $H_0 : \theta = \theta_0$, versus $H_1 : \theta = \theta_1 > \theta_0$,

$$k(\theta_1) = P(\text{Reject } H_0|H_1 \text{ true}) = P\left(\frac{(\bar{x}-\theta_0)\sqrt{n}}{S} > t_{\alpha/2}(n-1)\middle| H_1\right).$$

But under H_1,

$$P\left(\frac{\bar{x}-\theta_1+(\theta_1-\theta_0)\sqrt{n}}{S} > t_{\alpha/2}(n-1)\middle| H_1\right) =$$

$$P\left(\overbrace{\frac{(\bar{x}-\theta_1)\sqrt{n}}{S}}^{t-\text{dist under } H_1} + \overbrace{\frac{(\theta_1-\theta_0)\sqrt{n}}{S}}^{\text{If a constant, ok. } S \text{ is a rv}} > t_{\alpha/2}(n-1)\middle| H_1\right).$$

If $\theta = \theta_1$, then the distribution of $\frac{\sqrt{n}(\theta-\theta_0)}{S}$ is a *non-central t distribution* with a non-centrality parameter $\delta = \frac{\sqrt{n}(\theta_1-\theta_0)}{\sigma}$.

14.6.4 Testing About the Means of Two Normals

The random variables x and y have the following distributions $x \sim N(\mu_1, \sigma_1^2)$ and $y \sim N(\mu_2, \sigma_2^2)$. Assume that $\sigma_1 = \sigma_2 = \sigma$ if unknown. $x_1, x_2, ..., x_n$ is the random sample for x and $y_1, y_2, ..., y_m$ is the random sample for y. We have the following possible hypotheses tests. $H_0 : \mu_1 = \mu_2$ or $H_0 : \mu_1 - \mu_2 = 0$ versus $H_1 : \mu_1 > \mu_2$, $H_1 : \mu_1 < \mu_2$, or $H_1 : \mu_1 \neq \mu_2$. An estimator of $\mu_1 - \mu_2$ is $\bar{x} - \bar{y}$. $\bar{x} - \bar{y} \sim N\left(0, \sigma^2\left[\frac{1}{n} + \frac{1}{m}\right]\right)$. The pooled variance is $S_p^2 = \frac{(n-1)S_x^2+(m-1)S_y^2}{n+m-2}$. The test statistic is $T = \frac{(\bar{x}-\bar{y})}{S_p\sqrt{\frac{1}{n}+\frac{1}{m}}} \sim t(n+m-2)$.

For H_1	Reject If
$\mu_1 > \mu_2$	$T > t_\alpha(n+m-2)$
$\mu_1 < \mu_2$	$T < -t_\alpha(n+m-2)$
$\mu_1 \neq \mu_2$	$\lvert T\rvert > t_{\alpha/2}(n+m-2)$

The statistical power will be a non-central t distribution.

14.6.5 p-value

Example: $x \sim N(\mu, \sigma^2)$ and σ is known. We wish to test $H_0 : \mu = \mu_0$ versus $H_1 : \mu > \mu_0$. The test statistic is $z = \frac{\sqrt{n}(\bar{x}-\mu_0)}{\sigma}$. We reject H_0 if $z > z_\alpha$. Let z be the value of Z for a given random sample. $p = P(Z > z|H_0)$. If $\alpha > p$, then reject H_0 for this α. p is the smallest value of α for which we reject H_0. The smaller p is, the more significant the results. The probability of getting a value in the critical range is more extreme than z.

14.6.6 Testing About Variances

Suppose $x \sim N(\mu, \sigma^2)$. We wish to test $H_0 : \sigma = \sigma_0$ versus $H_1 : \sigma > \sigma_0$. S^2 is an unbiased estimator for σ^2. $\frac{(n-1)S^2}{\sigma_0^2} \sim \chi^2(n-1)$ under H_0. Under H_1,

$$\frac{(n-1)S^2}{\sigma_0^2} = \overbrace{\frac{(n-1)S^2}{\sigma_1^2}}^{\chi^2 \text{ under } H_1} \times \overbrace{\frac{\sigma_1^2}{\sigma_0^2}}^{\text{Constant}} > \frac{(n-1)S^2}{\sigma_1^2} \sim \chi^2.$$

We reject H_0 if $\frac{(n-1)S^2}{\sigma_0^2} > \chi^2_\alpha(n-1)$.

14.7 Chi-Square Goodness of Fit Test

Assume that the random variable x has some distribution with the pdf $f(x|\theta)$. Use a goodness-of-fit test for the assumed distribution.

Multinomial Distribution

Let $(n_1, n_2, ..., n_k) \sim Mulitnomial(n, p_1, p_2, ..., p_k)$. The pdf is given by $f(n_1, n_2, ..., n_k|\underline{p}) = \frac{n!}{\prod_{i=1}^k n_i!} \prod_{i=1}^k p_i^{n_i}$, where $\sum p_i = 1$ and $\sum n_i = n$. That is a $k-1$ dimensional random variable. Find the mle of p_i by maximizing f with respect to p_i. $\frac{d \log f}{dp_i} = \frac{n_i}{p_i} = 0$ does not work! Replace $p_k = 1 - \sum_{i=1}^{k-1} p_i$. Then, $\log f = c + \sum_{i=1}^{k-1} n_i \log p_i + n_k \log(1 - p_1 - p_2 - \cdots - p_{k-1})$. $\frac{d \log f}{dp_i} = \frac{n_i}{p_i} - \frac{n_k}{1-p_1-p_2-\cdots-p_{k-1}} = 0$. $\frac{n_i}{p_i} = \frac{n_k}{p_k} \Rightarrow n_i = \frac{n_k p_i}{p_k}$. Then, $\sum_{i=1}^k n_i = \frac{n_k}{p_k} \sum_{i=1}^k p_i \Rightarrow p_k = \frac{n_k}{n} \Rightarrow p_i = \frac{n_i}{n} \Rightarrow \widehat{p}_i = \frac{n_i}{n}$. $n_i \sim Binomial(n, p_i)$, $E(\widehat{p}_i) = \frac{1}{n} E(n_i) = \frac{np_i}{n} = p_i$, $Var(\widehat{p}_i) = \frac{1}{n^2} Var(n_i) = \frac{p_i(1-p_i)}{n}$ $Cov(n_i, n_j) = E(n_i n_j) - E(n_i)E(n_j) = -np_ip_j$. The covariance formula must be proven for homework.

The χ^2 Goodness of Fit Test

Let $(n_1, n_2, ..., n_k) \sim Multinomial(n, p_1, p_2, ..., p_k)$. Assume that $p_1, p_2, ..., p_k$ are known. $Q_{k-1} = \sum_{i=1}^k \frac{(n_i - np_i)^2}{np_i} = \sum_{i=1}^k \frac{(n_i - E(n_i))^2}{E(n_i)} \to \chi^2(k-1)$ as $n \to \infty$. If p_i^* is correct, then $E(n_i) \to np_i^*$. For the case $k = 2 : Q_1 = \frac{(n_1-np_1)^2}{np_1} + \frac{(n_2-np_2)^2}{np_2}$. $p_1 + p_2 = 1 \Rightarrow p2 = 1 - p_1$. $n_1 + n_2 = n \Rightarrow n_2 = n - n_1$. Then, $Q_1 = \frac{(n_1-np_1)^2}{np_1} + \frac{[n-n_1-n(1-p_1)]^2}{n(1-p_1)} = \frac{(n_1-np_1)^2}{np_1(1-p_1)} \to \chi^2(1)$ because $n_1 \sim Binomial(n, p_1)$. Compare Q_{k-1} with $\chi^2(k-1)$. Reject the null hypothesis that the $p_i's$ are the correct multinomial probabilities if $Q_{k-1} > \chi^2_\alpha(k-1)$. If $p_1, p_2, ..., p_k$ are not correct, then $\frac{(n_i-np_i)^2}{np_i} = \frac{(np_i^*-np_i)^2}{np_i} = \frac{n(p_i^*-p_i)^2}{p_i}$.

Test If $x \sim U(0,1)$

To test if x is $U(0,1)$ based on a sample $x_1, x_2, ..., x_n$, where $f(x) = 1, 0 < x < 1$ with k classes of equal probability, create k classes. Classify $x_1, x_2, ..., x_n$ into a multinomial distribution. Then we get $n_1, n_2, ..., n_k$. Then the vector $(n_1, n_2, ..., n_k) \sim Multinomial(n, p_1, p_2, ..., p_k)$ where $p_i = \frac{1}{k}$. $Q_{k-1} = \sum_{i=1}^k \frac{(n_i-np_i)^2}{np_i} \to$

$\chi^2_\alpha(k-1)$.

Problems: k is arbitrary. We do not want a small value of k. However if k is too large, then $n_i \sim Binomial(n, p_i)$. $\frac{n_i - np_i}{\sqrt{np_i q_i}} \to N(0,1), i = 1, 2, ..., k$. We want p_i subject to $np_i \geq 5, i = 1, 2, ..., k$. Therefore, $5 \leq k \leq 20$. For larger n, you can have larger k. $p_i = \int_{c_i - 1}^{c_i} dx$.

Suppose we want to test $H_0 : x \sim Exp(\theta)$, where θ is known. $f(x|\theta) = \frac{1}{\theta} e^{-\frac{x}{\theta}}$. Let $x_1, x_2, ..., x_n$ be the random sample. $p_i = P(c_{i-1} < x < c_i) = \int_{c_i - 1}^{c_i} \frac{1}{\theta} e^{-\frac{x}{\theta}}\, dx$. Classify $x_1, x_2, ..., x_n$ into a multinomial distribution. $Q_{k-1} = \sum_{i=1}^{k} \frac{(n_i - np_i)^2}{np_i}$

Suppose that $H_0 : x \sim Poisson(\theta)$.

x	0	1	2	$\cdots$	x
$f(x\|\theta)$	$e^{-\theta}$	$\theta e^{-\theta}$	$\frac{\theta^2 e^{-\theta}}{2!}$	$\cdots$	$\frac{\theta^x e^{-\theta}}{x!}$

which assumes that θ is known. If $x_1, x_2, ..., x_n$ is a random sample, then

Sample	$f(0)$	$f(1)$	$f(2)$	$\cdots$	$f(x)$
$nf(x\|\theta)$	$ne^{-\theta}$	$n\theta e^{-\theta}$	$\frac{n\theta^2 e^{-\theta}}{2!}$	$\cdots$	$\frac{n\theta^x e^{-\theta}}{x!}$

Whenever combining $nf(x|\theta) > 5$, stop combining and start a new classification. $(n_1, n_2, ..., n_k) \sim Multinomial(n, p_1, p_2, ..., p_k)$, $\sum_{i=1}^{k} \frac{(n_i - np_i)^2}{np_i} \to \chi^2_\alpha(k-1)$.

14.7.1 The Chi-Square Test When the Parameters Are Unknown

Let x have the pdf $f(x|\theta)$ where θ is

$$\theta = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_r \end{pmatrix}$$

is a vector of unknown parameters. $x_1, x_2, ..., x_n$ is the random sample.

$$p_i(\theta) = \int_{c_{i-1}}^{c_i} f(x|\theta)\, dx, \;\; Q_{k-1} = \sum_{i=1}^{n} \frac{(n_i - np_i(\theta))^2}{np_i(\theta)}$$

is not a test statistic because θ is unknown. The data is $n_1, n_2, ..., n_k$ and $\widehat{p_i} = \frac{n_i}{n}, i = 1, 2, ..., k-1$ is meaningless because there are too many parameters to estimate. We need an estimator of θ.

1. We can use the MLE based on the $x_1, x_2, ..., x_n$ random sample. Call it $\widehat{\theta}$. It maximizes $L = \prod_{i=1}^{n} f(x_i|\theta)$.

2. We can use the MLE based on $Multinomial(n, p_1, p_2, ..., p_k)$. Call it $\widetilde{\theta}$. It maximizes $L^* = c \prod_{i=1}^{k} p_i^{n_i}(\theta)$.

3. We can use the minimum chi-square estimator. Call it $\widehat{\theta}^*$. $\widehat{Q}_{k-1}(\theta = \widehat{\theta}^*) \leq Q_{\theta\in\Omega}(k-1)$. Then use, $\widehat{Q}_{k-1}(\widetilde{\theta}) \to \chi^2(k-r-1)$ as $n \to \infty$. and $\widehat{Q}_{k-1}(\widehat{\theta}^*) \to \chi^2(k-r-1)$ as $n \to \infty$. We can also use $\widehat{Q}_{k-1}(\widehat{\theta}) \to \chi^2(k-r-1) + \lambda_1 x_1^2 + \lambda_2 x_2^2 + \cdots + \lambda_r x_r^2$.

Suppose we test $H_0 : x \sim N(\theta_1, \theta_2^2)$. $\widehat{\theta}_1 = \bar{x}$, $\widehat{\theta}_2 = S$, where $S^2 = \frac{1}{n}\sum_{i=1}^n (x_i - \bar{x})^2$. Then,

$$p_i(\theta) = \int_{c_{i-1}}^{c_i} \frac{1}{\sqrt{2\pi}\theta_2} e^{-\frac{(x-\theta_1)^2}{2\theta_2^2}}\, dx \text{ is wrong.}$$

Suppose we use $\widehat{\theta}$. If we do not reject H_0 based on $Q_{k-1}(\widehat{\theta})$, then we will not reject H_0 based on $Q_{k-1}(\widehat{\theta}^*)$. Using $\widehat{Q}_{k-1}(\widehat{\theta})$, inflates α.

14.7.2 Testing for Two Multinomial Distributions

Suppose that $x_{11}, x_{21}, ..., x_{k1} \sim Multinomial\ (n_1, p_{11}, p_{2,1}, ..., p_{k1})$ and that $x_{12}, x_{22}, ..., x_{k2} \sim Multinomial\ (n_2, p_{12}, p_{22}, ..., p_{k2})$. The null hypothesis is $H_0 : p_{i1} = p_{i2} = p_i, i = 1, 2, ..., k$. $Q = \sum_{i=1}^k \sum_{j=1}^2 \frac{(x_{ij} - n_j p_{ij})^2}{n_j p_{ij}} = \chi^2[2(k-1)]$ because

$$\overbrace{\frac{\sum (x_{i1} - n_1 p_{i1})^2}{n_1 p_{i1}}}^{\chi^2(k-1)} + \overbrace{\frac{\sum (x_{i2} - n_2 p_{i2})^2}{n_2 p_{i2}}}^{\chi^2(k-1)}$$

Under H_0, $Q = \sum_{j=1}^2 \sum_{i=1}^k \frac{(x_{ij} - n_j p_i)^2}{n_j p_i}$ but the $p_i's$ are unknown. Based on the joint pdf of the two samples, $\widehat{p}_i = \frac{x_{i1} + x_{i2}}{n_1 + n_2} = \frac{x_{i1} + x_{i2}}{n}, i = 1, 2, ..., k$. Then, $\widehat{Q} = \sum_{j=1}^2 \sum_{i=1}^k \frac{(x_{ij} - n_j \widehat{p}_i)^2}{n_j \widehat{p}_i} \to \chi^2(r)$ where $r = 2k - 2 - (k-1) = k-1$.

Example: Let $x_1, x_2, ..., x_{n_1}$ be a random sample from the distribution $N(\theta_{11}, \theta_{21}^2)$, and $y_1, y_2, ..., y_{n_2}$ be a random sample from the distribution $N(\theta_{12}, \theta_{22}^2)$. We wish to test the hypothesis that both samples are from the same normal distribution or $H_0 : \theta_{11} = \theta_{12} = \theta_1$ *and* $\theta_{21} = \theta_{22} = \theta_2$.

$$p_i(\theta) = \int \frac{1}{\sqrt{2\pi}\theta_2} e^{-\frac{(x-\theta_1)^2}{2\theta_2^2}}\, dx.$$

We only need to estimate the pair (θ_1, θ_2).

$$\widehat{Q} = \sum_{j=1}^{2} \sum_{i=1}^{k} \frac{(x_{ij} - n_j p_i(\widehat{\theta}))^2}{n_j p_i(\widehat{\theta})} \to \chi^2(r), r = 2k - 2 - 2 = 2k - 4.$$

14.7.3 Independence of Two Attributes

This section pertains to a contingency table analysis. Suppose there is a Factor A at a levels and a Factor B at b levels. Then, we have the following table.

	1	2	$\cdots$	j	$\cdots$	b	
1				p_{1j}			
2							
$\vdots$							
i	p_{i1}	p_{i2}	$\cdots$	p_{ij}	$\cdots$	p_{ib}	$p_{i\cdot}$
$\vdots$				$\vdots$			
a	$\cdots$	$\cdots$	$\cdots$	p_{aj}	$\cdots$	$\cdots$	
				$p_{\cdot j}$			

There are n objects to be classified into $a \times b = k$ classes. x_{ij} = number in the $(i,j)^{th}$ class. $(x_{11}, ..., x_{ab}) \sim Multinomial$. $p_{ij} = P$(Subject belongs to the $(i,j)^{th}$ class). $Q = \sum_{i,j} \frac{(x_{ij}-np_{ij})^2}{np_{ij}} \rightarrow \chi^2(k-1)$. The null hypothesis tests whether the levels of Factor A are independent of the levels of Factor B. P(Subject belongs to A_i) $= \sum_j p_{ij} = p_{i\cdot}$. P(Subject belongs to B_j) $= \sum_i p_{ij} = p_{\cdot j}$. P(Subject lies in the $(i,j)^{th}$ class) $= p_{i\cdot}p_{\cdot j}$. The last probability is due to independence under the null hypothesis.

Example: Consider the two events smoking and cancer. $Q = \frac{(x_{ij}-np_{i\cdot}p_{\cdot j})^2}{np_{i\cdot}p_{\cdot j}}$. We need to estimate $p_{i\cdot}$ and $p_{\cdot j}$. $(x_{1\cdot}, x_{2\cdot}, ..., x_{a\cdot} \sim Multinomial(n, p_{1\cdot}, p_{2\cdot}, ..., p_{a\cdot})$. Then, $\widehat{p}_{i\cdot} = \frac{x_{i\cdot}}{n}$. Then,

$$\widehat{Q} = \sum \frac{(x_{ij} - n\widehat{p}_{i\cdot}\widehat{p}_{\cdot j})^2}{n\widehat{p}_{i\cdot}\widehat{p}_{\cdot j}} \rightarrow \chi^2(ab - 1 - (a - 1 + b - 1)) = \chi^2[(a-1)(b-1)]$$

where the number of parameters is $a - 1 + b - 1$.

14.8 Measures of Quality of Estimators

Let $\widehat{\theta}$ be an estimator of θ. We want $P(-a < \widehat{\theta} - \theta < a)$ to be high. This depends on the $E(\widehat{\theta})$ and the $Var(\widehat{\theta})$. If $E(\widehat{\theta}) = \theta$, then it is unbiased. If we restrict our estimators to be unbiased, then we can compare their variances.

Definition: $\widehat{\theta}$ is an *unbiased minimum variance estimator (UMVE)* of θ if $E(\widehat{\theta}) = \theta$ and $Var(\widehat{\theta}) \leq Var(\widetilde{\theta})$ for any other unbiased estimator $\widetilde{\theta}$. $Var(\widehat{\theta})$ is a *risk function.* $Var(\widehat{\theta}) = E(\widehat{\theta} - \theta)^2$ if $\widehat{\theta}$ is unbiased.

Loss Function	Risk Function
$\lvert\widehat{\theta} - \theta\rvert = L(\widehat{\theta}, \theta)$	$R(\widehat{\theta}, \theta) = E\lvert\widehat{\theta} - \theta\rvert$
$(\widehat{\theta} - \theta)^2 = L(\widehat{\theta}, \theta)$	$R(\widehat{\theta}, \theta) = E(\widehat{\theta} - \theta)^2$

The second entry in the above table is called the *mean square error* of $\widehat{\theta}$.

Example: $x \sim N(\theta, 1)$. $\widehat{\theta} = \bar{x}$. $E(\widehat{\theta} - \theta)^2 = \frac{1}{n} = MSE(\widehat{\theta})$. Choose $\widetilde{\theta} = 0$. Then, the $MSE(\widetilde{\theta}) = \theta^2$.

Example: $n = 16$. For $-\frac{1}{4} < \theta < \frac{1}{4}, MSE(\widetilde{\theta}) < MSE(\widehat{\theta})$. We want to restrict $\widehat{\theta}$ to the unbiased class of estimators and the mini-max estimator.

Definition: Let the risk function $R(\widehat{\theta}, \theta) = E(\widehat{\theta} - \theta)^2$. $\widehat{\theta}$ is the *maximum estimator* of θ if $\max_{\theta \in \Omega} R(\widehat{\theta}, \theta) \leq \max_{\theta \in \Omega} R(\widetilde{\theta}, \theta)$ for any other estimator $\widetilde{\theta}$. The unbiased minimum variance estimator may or may not be the mini-max estimator. Suppose that $E(\widehat{\theta}) = \theta + b_n(\theta)$. Then, $E(\widehat{\theta} - \theta)^2 = E(\widehat{\theta} - \theta - b_n(\theta))^2 = E(\widehat{\theta} - \theta - b_n(\theta))^2 + b_n^2(\theta) + 2b_n(\theta)E(\widehat{\theta} - \theta - b_n(\theta))$. The $MSE(\widehat{\theta}) = Var(\widehat{\theta}) + b_n^2(\theta)$ because $2b_n(\theta)E(\widehat{\theta} - \theta - b_n(\theta)) = 0$.

Example: Total distances traveled versus the total squared distances.

```
----|-----|----------|----------|----
    x1    x2        theta         xn
```

1. $R(\theta) = \sum |x_i - \theta|$ is the total distance traveled by all n workers. R is minimized by $\theta = medain(x_1, x_2, ..., x_n)$.
2. $R(\theta) = \sum (x_i - \theta)^2$ is the total of the squared distances. R is minimized by $\theta = \bar{x}$ which is the arithmetic mean.

In fact, for random variable $E|x - \theta|$ is the minimum if $\theta = median(x)$ and $E(x - \theta)^2$ is the minimum if $\theta = E(x)$. Let $E(x) = \mu$. Then, $E(x - \theta)^2 = E(x - \mu + \mu - \theta)^2 = E(x - \mu)^2 + (\mu - \theta)^2 + 2(\mu - \theta)E(x - \mu) = E(x - \mu)^2 + (\mu - \theta)^2$. Then for any θ, $E(x - \theta)^2 \geq E(x - \mu)^2$.

14.9 Finding the Unbiased Minimum Variance Estimator

Example: Let $x \sim N(\theta, \sigma^2)$. $\widehat{\theta} = \bar{x}$ is unbiased. So is $\widetilde{\theta} = \sum_{i=1}^{n} a_i x_i, \sum a_i = 1$. How do we know that $\bar{x}$ is the NMVE?

Definition: If $P(x_1, x_2, ..., x_n|T)$ is independent of θ, then T is the *sufficient statistic* for θ. Here $T = T(x_1, x_2, ..., x_n)$. The joint pdf of $x \sim f(x|\theta)$ is

$$P(x_1, x_2, ..., x_n, \theta) = \prod_{i=1}^{n} f(x_i|\theta) = P(x_1, x_2, ..., x_n|T)g(T|\theta).$$

If $P(x_1, x_2, ..., x_n|T)$ does not depend on θ, then maximizing the likelihood function only involves maximizing $g(T|\theta)$.

$$P(x_1, x_2, ..., x_n|T) = \frac{P(x_1, x_2, ..., x_n, T, \theta)}{g(T|\theta)} = H(x_1, x_2, ..., x_n).$$

Example: $x \sim N(\theta, \sigma^2)$ and σ is known.

$$P(x_1, x_2, ..., x_n|\theta) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^n e^{-\frac{(x_i-\theta)^2}{2\sigma^2}}.$$

Note that $\sum(x_i - \theta)^2 = \sum(x_i - \bar{x} + \bar{x} - \theta)^2 = \sum(x_i - \bar{x})^2 + n(\bar{x} - \theta)^2$. Then,

$$\frac{1}{(\sqrt{2\pi}\sigma)^n} e^{-\frac{\sum(x_i-\bar{x})^2}{2\sigma^2}} e^{-\frac{n(\bar{x}-\theta)^2}{2\sigma^2}},$$

$\bar{x} \sim N(\theta, \sigma^2/n)$. $g(\bar{x}|\theta) = \frac{\sqrt{n}}{\sqrt{2\pi}\sigma} e^{-\frac{n(\bar{x}-\theta)^2}{2\sigma^2}}$. Then, $P(z_1, x_2, ..., x_n|\bar{x}) = \frac{P(x_1, x_2, ..., x_n|\theta)}{g(\bar{x}|\theta)} = ce^{-\frac{\sum(x_i-\bar{x})^2}{2\sigma^2}} \Rightarrow T = \bar{x}$ is *sufficient* for θ.

14.10 Factorization Theorem

Theorem: Assume that the range of x does not depend on θ. The test statistic $T = T(x_1, x_2, ..., x_n)$ is *sufficient* for θ iff $\prod_{i=1}^{n} f(x_i|\theta) = k_1(t, \theta)h(\underline{x})$, where $h(\underline{x})$ does not depend on θ.

Proof: Transform $x_1, x_2, ..., x_n$ to $t, y_1, y_2, ..., y_{n-1}$. Then,

$$g(t|\theta) = \int k(t, \theta)h(t, y_1, y_2, ..., y_{n-1}|J)\, dy_1, ..., dy_{n-1} = k(t, \theta)c(t).$$

$$P(x_1, x_2, ..., x_n|t) = \frac{P(x_1, x_2, ..., x_n, t)}{P(t|\theta)} = \frac{k(t, \theta)h(\underline{x})}{k(t, \theta)c(t)} = \frac{h(\underline{x})}{c(t)}.$$

Example: $x_1, x_2, ..., x_n$ is a random sample from $Poisson(\theta)$.

$$\prod_{i=1}^{n} f(x_i|\theta) = \prod_{i=1}^{n} \frac{e^{-\theta}\theta^{x_i}}{x_i!} = e^{-n\theta}\theta^{n\bar{x}} \left(\frac{1}{\prod_{i=1}^{n} x_i!}\right) \Rightarrow$$

$\bar{x}$ is a sufficient statistic for θ and $t = \sum x_i$ is sufficient for θ. One is the function of another.

Example: Find the sufficient statistics for $x \sim Gamma(\theta_1, \theta_2)$. If

$$t = \begin{pmatrix} t_1 \\ t_2 \\ \vdots \\ t_m \end{pmatrix}, \theta = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_k \end{pmatrix}.$$

t is sufficient for θ iff $\prod_{i=1}^{n} f(x_i|\theta) = g(t, \theta)h(\underline{x})$ for $m \geq k$ or $m < k$. $f(x|\theta) = \frac{e^{-\frac{x}{\theta_1}} x^{\theta_2 - 1}}{\theta_1^{\theta_2}\Gamma(\theta_2)}$.

$$\prod_{i=1}^{n} f(x_i|\theta) = \prod_{i=1}^{n} \frac{e^{-\frac{x_i}{\theta_1}} x_i^{\theta_2-1}}{\theta_1^{\theta_2}\Gamma(\theta_2)} = \frac{e^{-\frac{\sum x_i}{\theta_1}} (\prod x_i)^{\theta_2-1}}{\theta_1^{n\theta_2}\Gamma(\theta_2)^n} = \frac{e^{-\frac{t_1}{\theta_1}} t_2^{\theta_2-1}}{\theta_1^{n\theta_2}\Gamma(\theta_2)^n} \times 1.$$

by letting $t_1 = \sum x_i$ and $t_2 = \prod x_i$. Note that $h(\underline{x}) = 1$ here which implies (t_1, t_2) are jointly sufficient for (θ_1, θ_2).

Example: Consider the case when the range of x depends on θ. $f(x|\theta) = \frac{1}{\theta}, 0 < x < \theta$. Show $x_{(n)}$ is a sufficient statistic. $g(x_{(n)}|\theta) = \frac{nx_{(n)}^{n-1}}{\theta^n}, 0 < x_{(n)} < \theta$. The distribution of $(x_1, x_2, ..., x_n)|x_{(n)}$ must be independent of θ.

$$P(x_1, x_2, ..., x_n|x_{(n)}) = \frac{P(x_1, x_2, ..., x_n, x_{(n)})}{g(x_{(n)}|\theta)} = \frac{\left(\frac{1}{\theta^n}\right)}{\frac{nx_{(n)}^{n-1}}{\theta^n}} = \frac{1}{nx_{(n)}^{n-1}}, 0 < x_i < x_{(n)}.$$

The joint distribution does not depend on θ. Therefore, $x_{(n)}$ is a sufficient statistic by the original definition.

Example: $x \sim N(\mu, \sigma^2)$. The likelihood function is

$$\prod_{i=1}^{n} f(x_i|\mu, \sigma^2) = \frac{e^{-\frac{\sum_{i=1}^{n}(x_i-\mu)^2}{2\sigma^2}}}{(\sqrt{2\pi}\sigma)^n},$$

$$\sum_{i=1}^{n}(x_i - \mu)^2 = \sum_{i=1}^{n}(x_i - \bar{x} + \bar{x} - \mu)^2 = \sum_{i=1}^{n}(x_i - \bar{x})^2 + \sum_{i=1}^{n}(\bar{x} - \mu)^2.$$

Then, the likelihood function becomes

$$\frac{e^{-\frac{\sum_{i=1}^{n}(x_i-\bar{x})^2 + n(\bar{x}-\mu)^2}{2\sigma^2}}}{(\sqrt{2\pi}\sigma)^n}.$$

1. If σ is known, then $g(\bar{x}, \mu)h(\underline{x}, \sigma) \Rightarrow \bar{x}$ is sufficient for μ by the second likelihood function.

2. If μ is known, then $t = \sum_{i=1}^{n}(x_i - \mu)^2$ is sufficient by the first likelihood function.

$$\widehat{\sigma}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2, \;\; \widetilde{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2,$$

   Both are unbiased since $E(\widehat{\sigma}^2) = E(\widetilde{\sigma}^2) = \sigma^2$. t is better because it is sufficient and $Var(\widetilde{\sigma}^2) < Var(\widehat{\sigma}^2)$.

3. If both μ and σ are unknown, the using the second likelihood function, $t_1 = \sum_{i=1}^{n}(x_i - \bar{x})^2$ and $t_2 = \bar{x} \Rightarrow$

$$L = g(t_1, t_2, \mu, \sigma) = \frac{1}{(\sqrt{2\pi}\sigma)^n} e^{-\frac{t_1 + n(t_2-\mu)^2}{2\sigma^2}}.$$

Example: $f(x|\theta) = \frac{\theta}{(e^{\theta^2}-1)}, e^{\theta x}, 0 < x < \theta$. $\prod_{i=1}^{n} f(x_i|\theta) = \frac{\theta^n}{(e^{\theta^2}-1)^n} e^{\theta \sum x_i}$. We can not use the factorization theorem because of the range. If $t_1 = \sum x_i$ and $t_2 = x_{(n)}$. Then, (t_1, t_2) are jointly sufficient for θ.

14.11 Sufficiency When the Range of x Depends on θ

We have $f(x|\theta), a(\theta) < x < b(\theta)$. $\prod_{i=1}^{n} f(x_i|\theta), a(\theta) < x_i < b(\theta), i = 1, 2, ..., n$. The ordered sample is $x_{(1)} < x_{(2)} < \cdots < x_{(n)}$. Define $A = \{\underline{x} : a(\theta) < x_{(1)} < \cdots < x_{(n)} < b(\theta)\} = \{\underline{x} : a(\theta) < x_i < b(\theta)\}$.

$$I_A(x_{(1)}, x_{(n)}, \theta) = \begin{cases} 1, & \text{if } \underline{x} \in A. \\ 0, & \text{otherwise.} \end{cases}$$

$$\prod_{i=1}^{n} f(x_i|\theta) = \prod f(x_i|\theta) I_A(x_{(1)}, x_{(n)}, \theta), -\infty < x_i < \infty, i = 1, 2, ..., n.$$

Now we can use the Factorization Theorem.

1. If $f(x_i|\theta)$ is just a function of θ, then $L = g(x_{(1)}, x_{(n)}, \theta)u(\theta)$. This implies $x_{(1)}$ and $x_{(n)}$ are sufficient for θ.

2. Suppose we just have the sample $(x_1, x_2, ..., x_n)$. Define $A = \{\underline{x} : 0 < x_{(n)} < \theta\}$ and

$$I_A(x_{(n)}, \theta) = \begin{cases} 1, & \text{if } \underline{x} \in A. \\ 0, & \text{otherwise.} \end{cases}$$

   Then,

$$L = \frac{\theta^n}{(e^{\theta^2}-1)^n} e^{\theta \sum x_i} I_A(x_{(n)}, \theta), -\infty < x_i < \infty.$$

   We can conclude that $\sum x_i$ and $x_{(n)}$ are sufficient statistics for θ because they cannot be separated from θ.

14.11.1 Results Related to Sufficient Statistics

1. If t_1 is sufficient for θ and if t_2 is also sufficient for θ, then t_1 and t_2 must be functionally related. $t_1 = t_1(x_1, x_2, ..., x_n)$ and $t_2 = t_2(x_1, x_2, ..., x_n)$. If t_1 is sufficient, then the conditional distribution of t_2 given t_1 $g_2(t_2|t_1)$ is independent of θ since $(x_1, x_2, ..., x_n|t_1)$ is independent of θ by the definition of sufficiency. If t_2 is sufficient, then $g_4(t_1|t_2)$ is independent of θ. $g(t_1, t_2|\theta) = g_1(t_1|\theta)g_2(t_2|t_1)$ and $g(t_1, t_2|\theta) = g_3(t_2|\theta)g_4(t_1|t_2)$. Then, by division,

$$1 = \frac{g_1(t_1|\theta)g_2(t_2|t_1)}{g_3(t_2|\theta)g_4(t_1|t_2)} \Rightarrow \frac{g_3(t_2|\theta)}{g_1(t_1|\theta)} = \frac{g_2(t_2|t_1)}{g_4(t_1|t_2)}.$$

   Since the second part of the above equality is independent of θ then the first part of the equality must be independent also. This implies that the set (t_1, t_2) is a function of each other. That is, $t_1 = u(t_2)$.

   Example: Suppose we hat $x \sim Poisson(\theta)$. $t_1 = \sum x_i$ is sufficient for θ. $t_2 = \bar{x}$ is also sufficient for θ. But, $t_2 = \frac{t_1}{n}$.

2. If t_1 is sufficient for θ, then any one-to-one function of t_1 is also sufficient for θ where the range does not depend on θ. The mle of θ is a function of sufficient statistics. Let x have the pdf $f(x|\theta)$. If t is sufficient for θ, $L(\theta|\underline{x}) = \prod_{i=1}^n f(x_i|\theta) = g(t,\theta)h(\underline{x})$, $\frac{d\log L}{d\theta} = \frac{d\log g(t,\theta)}{d\theta} = 0 \Rightarrow \widehat{\theta} = u(t)$.

   In the multi-parameter case:

$$\theta = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_k \end{pmatrix} \text{ and } t = \begin{pmatrix} t_1 \\ t_2 \\ \vdots \\ t_m \end{pmatrix}.$$

   If t is sufficient for θ, then $L(\theta|\underline{x}) = \prod_{i=1}^n f(x_i|\theta) = g(t,\theta)h(\underline{x})$, $\frac{d\log L}{d\theta_i} = \frac{d\log g(t,\theta)}{d\theta_i} = 0, i = 1, 2, ..., k$.

   Example: When $x \sim N(\mu, \sigma^2)$, $L(\mu, \sigma^2|\underline{x}) = c\frac{1}{\sigma^2}e^{-\frac{t_1}{2\sigma^2} - \frac{n(t_2-\mu)^2}{2\sigma^2}}$, $t_1 = \sum(x_i - \bar{x})^2$, $t_2 = \bar{x}$. The mle's are $\widehat{\mu} = t_2 = \bar{x}$ and $\widehat{\sigma}^2 = \frac{1}{n}\sum(x_i - \bar{x})^2 = \frac{t_1}{n}$. The minimum unbiased variance estimator is $\widetilde{\sigma}^2 = \frac{t_1}{n-1}$ which is unbiased for σ^2. The next section will show how we know these are minimum unbiased variance estimators.

14.12 Rao-Blackwell Theorem

Homework Number 2: Chapter 7, 7.4, 7.7, 7.8, 7.17, 7.20, 7.25, 7.27, 7.37, 7.42, 7.46, 7.54, 7.61. For problem 7.13, let x be a continuous random variable with the density function $f(x)$. Prove that $E|x - \theta|$ is minimum if $\theta = median(x)$.

Rao-Blackwell Theorem: Let T_1 be a sufficient statistic for θ and let T_2 be an unbiased estimator of θ. Then, there exists a function $\psi_1(T_1)$ such that

1. $E[\psi(T_1)] = 0$ or $E[\psi(T_1)] = \phi(\theta)$ which is simply a function of θ.

2. $Var[\psi(T_1)] \leq Var(T_2)$. **Proof:** $\theta = E(T_2) = E_{T_1}[E(T_2|T_1)]$, $E(T_2|T_1 = t_1) = \int t_2 h(t_2|t_1)\, dt_2 = \psi(t_1)$. Then we have $E_{T_1}(\psi(t_1))$ implies results from (1). Moreover

$$Var(T_2) = E[T_2 - \theta]^2 = E[T_2 - \psi(T_1) + \psi(T_1) - \theta]^2 =$$

$$E[(T_2 - \psi(T_1))^2 + \overbrace{(\psi(T_1) - \theta)^2}^{Var(\psi(T_1)} + 2(\psi(T_1) - \theta)(T_2 - \psi(T_1)] = Var(\psi(T_1)) + E[T_2 - \psi(T_1)]^2,$$

$$E[(\psi(T_1) - \theta)(T_2 - \psi(T_1))] = E_{T_1}[(\psi(T_1) - \theta)\overbrace{E[(T_2 - \psi(T_1)|T_1]}^{=0}] = 0$$

Then, we have $Var(T_2) = Var(\psi(T_1)) + E[(T_2 - \psi(T_1))]^2 \Rightarrow Var(T_2) \geq Var(\psi(T_1))$. A general result in the text book shows that $\frac{Var(y)}{(Larger)}$ and $\frac{Var(y|x)}{(Smaller)}$. $Var(y) = E[Var(y|x)] + Var[E(y|x)] \Rightarrow Var(y) \geq Var[E(y|x)]$. Taking $y = T_2, x = T_1, E(T_2|T_1) = \psi(T_1), Var(T_2) \geq Var(\psi(T_1))$. **Proof:** $Var(y) = E[y - E(y)]^2 = E[y - E(y|x) + E(y|x) - E(y)]^2 = E[y - E(y|x)]^2 + E[E(y|x) - E(y)]^2 + 2E[(y - E(y|x))(E(y|x) - E(y))] = E_x[E(y - E(y|x))|x]^2 + E_x[E(E(y|x) - E(y))|x]^2 = E_x[Var(y|x)] + \cdots$

Example: Let $x_1, x_2, ..., x_n$ be a random sample from $Poisson(\theta)$. $\phi(\theta) = P(x = 0) = e^{-\theta}$. $T = \sum x_i$ is a sufficient statistic for θ.

$$T_1 = \begin{cases} 1, & \text{if } x_1 = 0. \\ 0, & \text{otherwise} \end{cases}$$

$E(T_1) = 1P(x_1 = 0) + 0P(x_1 > 0) = P(x_1 = 0) = e^{-\theta}$. We need to find $E(T_1|T)$ or find the distribution of $x_1|T$. $f(x_1, x_2, ..., x_n|\theta) = \prod_{i=1}^n \frac{e^{-\theta}\theta^{x_i}}{x_i!}$. $T = \sum_{i=1}^n x_i \sim Poisson(n\theta)$. Then,

$$g(x_1, x_2, ..., x_n|t) = \frac{g(x_1, x_2, ..., x_n, t)}{h(t|\theta)} = \frac{\frac{e^{-n\theta}\theta^{\sum_{i=1}^n x_i}}{\prod_{i=1}^n x_i!}}{\frac{e^{-n\theta}(n\theta)^t}{t!}} = \frac{t!}{\prod x_i!} \times \frac{1}{n^t} =$$

$$\frac{t!}{x_1! \cdots x_n!}\left(\frac{1}{n}\right)^{\sum_{i=1}^n x_i} \sim Multinomial\left(\frac{1}{n}, \frac{1}{n}, ..., t\right).$$

So, we can conclude that $(x_1, ..., x_n|t) \sim Multinomial\left(\frac{1}{n}, \frac{1}{n}, ..., t\right)$ and that $(x_1|t) \sim Binomial\left(\frac{1}{n}, t\right)$. Now we can find $E(T_1|t)$. $E(T_1|t) = 1P(x_1 = 0|t) = P(x_1 = 0|t) = \left(1 - \frac{1}{n}\right)^t = \psi(t)$. Then,

$$E[\psi(T)] = \sum \psi(t)\frac{e^{-n\theta}(n\theta)^t}{t!} = \sum\left(1 - \frac{1}{n}\right)^t \frac{e^{-n\theta}(n\theta)^t}{t!} = e^{-n\theta}\sum_{t=0}^{\infty}\frac{[(n-1)\theta]^t}{t!} = e^{-n\theta}e^{(n-1)\theta} = e^{-\theta} \Rightarrow \text{ unbiased.}$$

14.13 Complete Family

Definition: Let $g(t|\theta)$ be the pdf of $T, \theta \in \Omega$. The family is complete iff $E[u(T)] = \int_{-\infty}^{\infty} u(T)g(t|\theta)\,dt = 0, \forall\theta \Rightarrow u(T) = 0, \forall t$. This implies that no function of T has an expectation of zero without the function being identically zero. If $\psi(T)$ is unbiased for $\phi(\theta)$, and if $g(t|\theta)$ (the pdf of T) is complete, then there is only one unbiased estimator of θ.

Example: $x \sim Poisson(\theta)$. $g(x|\theta) = \frac{e^{-\theta}\theta^x}{x!}$. Here, g is a complete family. **Proof:** Let $u(x)$ be such that $E[u(x)] = 0, \forall\theta$. Then, we have

$$\sum_{x=0}^{\infty} u(x)g(x|\theta) = 0, \ \sum_{x=0}^{\infty} u(x)\frac{e^{-\theta}\theta^x}{x!} = 0, \ \sum_{x=0}^{\infty} \frac{u(\theta)}{x!}\theta^x = 0, \forall\theta \Rightarrow u(x) = 0, \forall x \Rightarrow$$

The Poisson distribution is a complete family. If $T = \sum x_i \sim Poisson(n\theta)$, then $g(t|\theta)$ is a complete family and $\psi(t) = \left(1 - \frac{1}{n}\right)^t$ is unbiased for $\phi(\theta) = e^{-\theta}$. Can there be another function $\psi^*(t)$ which is unbiased for θ? No. If $\psi^*(t)$ was unbiased, then $E[\psi(t) - \psi^*(t)] = 0 \Rightarrow \psi(t) - \psi^*(t) = 0, \forall t$ because $g(t|\theta)$ is complete. Therefore, $\psi(t) = \psi^*(t), \forall t$ and furthermore, $\psi(t)$ is the unbiased minimum variance estimator of $\phi(\theta)$.

Result: If T is a sufficient and complete statistic for θ, then $\psi(T)$ is the unbiased, minimum variance estimator for $E[\psi(T)]$.

14.13.1 The Laplace Transform

The Laplace transform of $u(x)$ is given by $\int_0^{\infty} u(x)e^{-tx}\,dx = \psi(t)$. Then, $\psi(t)$ is the Laplace transform of $u(x)$. If $\psi(t) = 0, \forall t$, then $u(x) = 0, \forall x$.

Example: Consider the exponential family $x \sim Exponential(\theta)$. $g(x|\theta) = \frac{1}{\theta}e^{-x/\theta}, x > 0$. Let $u(x)$ be such that $E[u(x)] = 0$. Then,

$$\int_0^{\infty} u(x)\frac{1}{\theta}e^{-x/\theta}\,dx = 0, \forall\theta \Rightarrow \int_0^{\infty} u(x)e^{-tx}\,dx = 0, \forall t = \frac{1}{\theta} \Rightarrow$$

by the Laplace transform, $u(x) = 0, \forall x \Rightarrow g(x|\theta)$ is a complete family.

14.14 Implications of Complete Sufficient Statistics

Let t be a complete sufficient statistic for θ. If $\phi(t)$ is an unbiased estimator for $\psi(\theta)$, then it is a unique unbiased estimator of $\psi(\theta)$ as a function of t. This implies that $\phi(t)$ is the unbiased minimum variance estimator of $\psi(\theta)$.

Example: $x \sim Poisson(\theta)$. $t = \sum x_i$ is a complete sufficient statistic for θ. $\psi(\theta) = e^{-\theta}$, $\phi(t) = \left(1 - \frac{1}{n}\right)^t$ is the unbiased minimum variance estimator.

Example: $x_1, x_2, ..., x_n$ are iid Bernoulli random variables. $T = \sum x_i$ is *binomial*(n, θ). T is sufficient for θ. $g_T(t|\theta) = \begin{pmatrix} n \\ t \end{pmatrix}\theta^t(1-\theta)^{n-t}$. Let $u(t) \to E(u(T)) = 0$,

$$E[u(T)] = \sum u(t)\begin{pmatrix} n \\ t \end{pmatrix}\theta^t(1-\theta)^{n-t} = \sum u(t)\begin{pmatrix} n \\ t \end{pmatrix}\left(\frac{\theta}{1-\theta}\right)^t = 0.$$

Then, $\phi(\theta) = \frac{\theta}{1-\theta}$. Then,

$$\sum u(t)\begin{pmatrix} n \\ t \end{pmatrix}\phi^t = 0 \Rightarrow u(t) = 0, \forall t.$$

Suppose we are interested in $\widehat{\theta} = \frac{T}{n}$. It is the unbiased minimum variance estimator of θ. $E(\widehat{\theta}) = \theta$. $\psi(\theta) = Var(\widehat{\theta}) = \frac{\theta(1-\theta)}{n}$. $\phi(T) = \frac{\widehat{\theta}(1-\widehat{\theta})}{n}$. It is the unbiased minimum variance estimator of $\psi(\theta)$. The mle of $\psi(\theta)$ is $\psi(\widehat{\theta})$ $\psi(\widehat{\theta}) = \frac{\widehat{\theta}(1-\widehat{\theta})}{n}$.

14.14.1 The Exponential Family

Given the likelihood function of the form $L(\theta|\underline{x}) = \prod f(x_i|\theta) = \exp\{p(\theta)\sum k(x_i) + \sum s(x_i) + nq(\theta)\}$. Let $t = \sum k(x_i)$. Then, $L(\theta|\underline{x}) = \exp\{tp(\theta) + nq(\theta)\}\exp\{\sum s(x_i)\}$. This implies that t is sufficient for θ. Let $f(x|\theta)$ be the pdf of x. If $f(x|\theta) = \exp\{p(\theta)k(x) + s(x) + q(\theta)\}, a < x < b$,

1. a and b do not depend on θ.
2. $p(\theta)$ is a non-trivial function of θ.
3. $k'(x) \neq 0$ and $s(x)$ are both continuous functions of x.

If (1) - (3) hold true for the continuous random variable x, then f belongs to the class of the *exponential family.* For discrete distributions, replace (3) by "$k(x)$ is a non-trivial function of x on the set $\{x : x = a_1, a_2, ...\}$."

Theorem: $T = \sum_{i=1}^n k(x_i)$ is a complete sufficient statistic if $f(x|\theta)$ belongs to the class of the exponential family.

Example: $x \sim Poisson(\theta)$. $f(x|\theta) = \frac{e^{-\theta}\theta^x}{x!}$. Take $\theta^x = e^{x\log\theta}$ and $x! = e^{\log x!}$. Then, $\exp\{-\theta + x\log\theta - \log x!\}$ which implies that $T = \sum_{i=1}^n x_i$ is a complete sufficient statistic.

Example: $x \sim Bernoulli(\theta)$.

$$f(x|\theta) = \theta^x(1-\theta)^{1-x} = \left(\frac{\theta}{1-\theta}\right)^x (1-\theta) = \exp\left\{x\log\left(\frac{\theta}{1-\theta}\right) + \log(1-\theta)\right\}$$

which implies that $T = \sum_{i=1}^n x_i$ is a complete sufficient statistic.

Example: $x \sim N(0, \theta)$.

$$f(x|\theta) = \frac{1}{\sqrt{2\pi}\theta}e^{-\frac{x^2}{2\theta^2}} = \exp\left\{-\frac{x^2}{2\theta^2} - \frac{1}{2}\log\theta - \frac{1}{2}\log 2\pi\right\}.$$

$k(x) = x^2 \Rightarrow T = \sum x_i^2$ is a complete sufficient statistic. Also, $k^*(x) = \frac{x^2}{2} \Rightarrow T^* = \sum \frac{x_i^2}{2}$ is a complete sufficient statistic. **Proof:**

$$E[u(x)] = \int u(x)\exp\{p(\theta)k(x) + s(x) + q(\theta)\}\,dx = \int e^{s(x)}u(x)e^{p(\theta)k(x)}\,dx = 0.$$

Let $t = -p(\theta)$. Then, we have

$$\int e^{s(x)}u(x)e^{-tk(x)}\,dx = 0, \text{ let } y = k(x),$$

$$\int J \overbrace{e^{s^*(y)}}^{\text{can't be 0}} u[k^{-1}(y)]e^{-ty}\,dy = 0 \Rightarrow u(x) = 0, \forall x.$$

Example: $f(x|\theta) = \theta x^{\theta-1}, 0 < x < 1$. $f(x|\theta) = e^{(\theta-1)\log x + \log\theta}$ which implies f belongs to a regular exponential family. Also, $T = \sum \log x_i$ is a complete sufficient statistic.

14.14.2 Factorization

$$L = \theta^n \left(\prod_{i=1}^{n} x_i\right)^{\theta-1}, \quad T^* = \prod_{i=1}^{n} x_i \text{ is sufficient.}$$

There is no contradiction with $T = \log T^*$. Consider the case of

$$\theta = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \vdots \\ \theta_k \end{pmatrix}, \quad f(x|\theta) = \exp\left\{\sum_{j=1}^{l} p_j(\theta)k_j(x) + s(x) + q(\theta)\right\}.$$

l can be $l \geq k$ or $l < k$. $T_j = \sum_{i=1}^n k_j(x_i), j = 1, 2, ..., l$. $(T_1, T_2, ..., T_l)$ is a set of complete sufficient statistics for $\theta' = (\theta_1, \theta_2, ..., \theta_k)$.

Example: $x \sim N(\theta_1, \theta_2)$. The range can not depend on θ to use the exponential family results.

$$f(x|\theta) = \frac{e^{-\frac{(x-\theta_1)^2}{2\theta_2}}}{\sqrt{2\pi\theta_2}} = \exp\left\{-\frac{x^2}{2\theta_2} + \frac{x\theta_1}{\theta_2} - \frac{\theta_1^2}{2\theta_2} - \frac{1}{2}\log(2\pi) - \frac{1}{2}\log\theta_2\right\}$$

The set (T_1, T_2) is a complete sufficient statistic for (θ_1, θ_2) where $T_1 = \sum_{i=1}^n x_i$ and $T_2 = \sum_{i=1}^n x_i^2$. The mle of θ_2 is

$$\widehat{\theta}_2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2 = \frac{1}{n}\sum_{i=1}^{n} x_i^2 - n\bar{x}^2 = \frac{T_2}{n} - \left(\frac{T_1}{n}\right)^2.$$

But,

$$\widetilde{\theta}_2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2 = \frac{1}{n-1}T_2 - \frac{n}{n-1}\left(\frac{T_1}{n}\right)^2 \Rightarrow \widetilde{\theta}_2 \text{ is the unbiased minimum variance estimator of } \theta_2.$$

Homework #2 is due Monday, March 2nd. For problem 14, let $x_1, x_2, ..., x_n$ be iid random variables with $E(x_i) = \mu$ and $Var(x_i) = \sigma^2$. Prove that $\bar{x}$ is the unbiased minimum variance estimator in the linear class $\sum a_i x_i + b$ where the $a_i's$ and $b's$ are constants. Prove that $b = 0$ and $a_i = \frac{1}{n}$.

Example: $x \sim N(\theta, 1)$. Find the unbiased minimum variance estimator for $\phi(\theta) = P(x \leq c)$, where c is a known constant.

$$\phi(\theta) = \int_{-\infty}^{c} \frac{e^{-\frac{(x-\theta)^2}{2}}}{\sqrt{2\pi}}\, dx.$$

$\bar{x}$ is a complete sufficient statistic for θ since it is in the exponential family of curves. So, the mle is

$$\phi(\theta) = \int_{-\infty}^{c} \frac{e^{-\frac{(x-\bar{x})^2}{2}}}{\sqrt{2\pi}} dx.$$

Let

$$u(x_i) = \begin{cases} 1, & \text{if } x_i < c. \\ 0, & \text{otherwise.} \end{cases}$$

Then, $E[u(x_i)] = 1P(x_i < x) = \phi(\theta)$ which is unbiased. Switch the $x_i's$ to x_1. We need the joint distribution of $(x_1, \bar{x})$. $E[u(x_1)|\bar{x}]$ is needed. $(x_1, \bar{x})$ has a bivariate normal distribution. $E(x_1) = E(\bar{x}) = \theta$. $Var(x_1) = 1$, and $Var(\bar{x}) = \frac{1}{n}$. $\rho = \frac{1}{\sqrt{n}}$. Recall that if $\begin{pmatrix} x \\ y \end{pmatrix} \sim$ Bivariate Normal(μ, Σ), then $y|x \sim N\left(\alpha + \beta(x - \mu_x), \sigma^2_{y|x}\right)$ where $\sigma^2_{y|x} = \sigma^2_y(1 - \rho^2)$, $\alpha = \mu_y$, and $\beta = \frac{\rho\sigma_y}{\sigma_x}$. Then, $x_1|\bar{x} \sim N\left(\bar{x}, \frac{n-1}{n}\right)$, $\theta + \frac{1}{\sqrt{n}}\sqrt{n}(\bar{x} - \theta) = \bar{x}$. Note that $x_1 \sim N(\theta, 1)$. So,

$$E[u(x_1)|\bar{x}] = P(x_1 < c|\bar{x}) = \int_{-\infty}^{c} \frac{e^{-\frac{(x_1-\bar{x})^2}{2(n-1)}}}{\sqrt{2\pi}\sqrt{\frac{n-1}{n}}} dx_1.$$

Write,

$$\frac{\sqrt{n}}{\sqrt{n-1}}(x_1 - \bar{x}) = z, \quad \int_{-\infty}^{\sqrt{\frac{n}{n-1}}(c-\bar{x})} \frac{e^{-\frac{z^2}{2}}}{\sqrt{2\pi}} dz = \Phi\left(\sqrt{\frac{n}{n-1}}(c - \bar{x})\right) = \widehat{\Phi}(\theta)$$

is the unbiased minimum variance estimator. The mle is $\phi(\widehat{\theta}) = \Phi(c - \bar{x})$.

14.14.3 Case of Several Parameters

Consider the exponential family where

$$\theta = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_k \end{pmatrix}, \quad f(x|\theta) = \exp\left\{\sum_{j=1}^{m} p_j(\theta)k_j(x) + s(x) + q(\theta)\right\}.$$

Then, $\sum_{i=1}^n k_1(x_i), \sum_{i=1}^n k_2(x_i), \cdots, \sum_{i=1}^n k_m(x_i)$ is a set of m complete sufficient statistics for $\theta_1, \theta_2, ..., \theta_k$ where $m \geq k$ or $m < k$.

Example: $x \sim N(\theta_1, \theta_2)$.

$$f(x|\theta) = \frac{1}{\sqrt{2\pi}\sqrt{\theta_2}} e^{-\frac{(x-\theta_1)^2}{2\theta_2}} = \exp\left\{-\frac{x^2}{2\theta_2} - \frac{\theta_1^2}{2\theta_2} + \frac{\theta_1 x}{\theta_2}\right\} \exp\left\{\frac{1}{2}\log(2\pi\theta_2)\right\}.$$

$k_1(x) = x, k_2(x) = x^2, T_1 = \sum x_i, T_2 = \sum x_i^2$ are a set of complete sufficient statistics for θ_1 and θ_2. We know that $E(\bar{x}) = \theta_1$, and $s^2 = \frac{1}{n-1}\sum(x_i - \bar{x})^2$. $E(s^2) = \theta_2$. Here, $\bar{x}$ and s^2 are unbiased minimum variance estimators for θ_1 and θ_2 respectively. Even if $\theta_1 = \theta_2$, we still need T_1 and T_2.

Example: Consider the distribution $Gamma(\theta_1, \theta_2)$.

$$f(x|\theta) = \frac{e^{-\frac{x}{\theta_1}} x^{\theta_2 - 1}}{\theta_1^{\theta_2}\Gamma(\theta_2)} = \exp\left\{-\frac{x}{\theta_1} + (\theta_2 - 1)\log x + q(\theta)\right\}$$

where $e^{q(\theta)} = \frac{1}{\theta_1^{\theta_2}\Gamma(\theta_2)}$. $T_1 = \sum x_i$, and $T_2 = \sum \log x_i$ is a set of complete sufficient statistics for θ_1 and θ_2. $\phi(\theta) = \theta_1\theta_2 = E(x) = \bar{x} \Rightarrow \bar{x}$ is the unbiased minimum variance estimator of $\phi(\theta)$ because $E(\bar{x}) = \theta_1\theta_2$.

14.14.4 Minimum Set of Sufficient Statistics

The set of random variables $(x_1, x_2, ..., x_n)$ is always a set of sufficient statistics for θ.

Definition: The minimum set of sufficient statistics are those that are sufficient for the parameters and are functions of any other set of sufficient statistic.

Example: Consider the normal distribution $N(\theta_1, \theta_2)$. $T_1 = \sum x_i, T_2 = \sum x_i^2$ is a minimum set of sufficient statistics.

Example: Consider the Chaucy distribution.

$$f(x) = \frac{c}{1 + (x - \theta)^2}, \quad L = \frac{c^n}{\prod_{i=1}^{n}(1 + (x_i - \theta)^2)}$$

implies that $(x_1, x_2, ..., x_n)$ is the minimum set of statistics.

Example: $f(x|\theta) = \frac{1}{2}, \theta - 1 < x < \theta + 1$.

$$L(\theta|\underline{x}) = \left(\frac{1}{2}\right)^n, \theta - 1 < x_{(1)} < \cdots < x_{(n)} < \theta + 1.$$

The mle is not unique.

```
L(theta)
  |
  |
  |
  |            ------------
  |            |          |
  |            |          |
  |            |  mle     |
  |-----------|----------|------------ theta
             y2-1       y1+1
```

$$L = \left(\frac{1}{2}\right)^n I_A(y_1) I_A(y_2)$$

where $y_1 = x_{(1)}$, and $y_2 = x_{(n)}$. Then, y_1 and y_2 are jointly sufficient for θ.

14.14.5 Ancillary Statistic

Definition: A statistic whose distribution does not depend on θ is known as an ancillary statistic for θ.

Example: $x \sim N(\theta, \sigma^2)$. S^2 is ancillary for θ. It has no information about θ.

14.14.6 Location Invariance Statistic

θ is a location parameter if $f(x|\theta)\,dx = f(x-\theta)\,dx$. The distribution of $y = x - \theta$ does not depend on θ. If u is such that $u(x_1 + d, x_2 + d, \cdots, x_n + d) = u(x_1, x_2, ..., x_n)$ then u is location in-variate.

Example: Suppose that $x \sim N(\theta, \sigma^2)$. $s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$ is location invariant and $x_{(n)} - x_{(1)}, \sum x_i - x_{(1)}$ are location invariant.

14.14.7 Scale Invariant

θ is a scale parameter if $f(x|\theta)\,dx = \frac{1}{\theta} f\left(\frac{x}{\theta}\right)\,dx$. Write $y = \frac{x}{\theta} = f(y)\,dy$. Then, a scale invariant statistic is defined as $u(cx_1, cx_2, ..., cx_n) = u(x_1, x_2, ..., x_n)$. Then, u is a scale invariant statistic.

Example:

$$\frac{\bar{x}}{s} = \frac{\frac{\sum_{i=1}^{n} x_i}{n}}{\sqrt{\sum_{i=1}^{n} \frac{(x_i - \bar{x})^2}{n-1}}} = \frac{\sum_{i=1}^{n} \frac{y_i}{n}}{\sqrt{\sum_{i=1}^{n} \frac{(y_i - \bar{y})^2}{n-1}}}$$

where $y_i = cx_i$. $\frac{x_1}{x_1 + x_2}$ or $\frac{x_{(1)}}{x_{(n)}}$ are all scale invariant.

14.14.8 Location and Scale Parameters

θ_1 and θ_2 are location and scale parameters if

$$f(x|\theta) = \frac{1}{\theta_2} f\left(\frac{x - \theta_1}{\theta_2}\right)\,dx.$$

Use $y = \frac{x - \theta_1}{\theta_2}$. Then, we have $f(y)\,dy$. If $u(cx_1 + d, ..., cx_n + d) = u(x_1, ..., x_n)$, then u is a location and scale invariant statistic.

Example: $\frac{x_i - \bar{x}}{s}$ is location and scale invariant. $\frac{x_i - x_j}{s}$ is location and scale invariant. $\frac{x_{(n)} - x_{(1)}}{s}$ is location and scale invariant.

14.15 Baysian Estimation

Lecture 12 on February 25, 1998 is missing.

The posterior of θ is $k(\theta|\underline{x}) \propto g(y|\theta)h(\theta)$ if y is a sufficient statistic.

14.15.1 Loss Functions

Let $\delta(\underline{x})$ be an estimator of θ. Ł$[\delta(\underline{x}, \theta)]$ is the loss function. Find $E_\theta[$Ł$(\delta(\underline{x}, \theta))]$. We need to find the δ that minimizes $E_\theta[$Ł$(\delta(\underline{x}, \theta))]$.

Example: Let y be a sufficient statistic for θ. $\delta(y)$ is an estimator of θ. $Ł(\delta,\theta) = [\theta - \delta(y)]^2$. $E[Ł(\delta,\theta)] = E_\theta[\theta - \delta(y)]^2$. $E(\theta|y) = u(y)$ minimizes $E_\theta[\theta - \delta(y)]^2$.

$$E_\theta[\theta - u(y) + u(y) - \delta(y)]^2 = E[\theta - u(y)]^2 + \overbrace{[u(y) - \delta(y)]^2}^{\text{a constant}} + \overbrace{2[u(y) - \delta(y)]E_\theta(\theta - u(y))}^{=0}.$$

Therefore, it is minimum if $\delta(y) = u(y) = E(\theta|y)$. $h(\theta|y) = cg(y|\theta)h(\theta) = c\int \theta h(\theta)g(y|\theta)d\theta = u(y)$ is Baye's Posterior mean. If $Ł(\gamma,\theta) = |\theta - \gamma|$, then $E|\theta - \gamma|$ is minimum if $\delta = median(\theta, y)$.

Example: Let $x_1, x_2, ..., x_n$ be a random sample from $Bernoulli(\theta)$. $y = \sum_{i=1}^n x_i \sim Binomial(n,\theta)$ is sufficient for θ. $g(y|\theta) = \left(\begin{array}{c} n \\ y \end{array}\right)\theta^y(1-\theta)^{n-y}$. The prior distribution is $\theta \sim Beta(\alpha,\beta)$. $f = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{\Gamma(\alpha,\beta)}$, $\beta(\alpha,\beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}$. $E(x) = \frac{\alpha}{\alpha+\beta}$. Then, $h(\theta) = \frac{\theta^{\alpha-1}(1-\theta)^{\beta-1}}{\beta(\alpha,\beta)}$ is prior. The posterior distribution is $k(\theta|y) = c\theta^y(1-\theta)^{n-y}\theta^{\alpha-1}(1-\theta)^{\beta-1} = c\theta^{y+\alpha-1}(1-\theta)^{n-y+\beta-1}$. Then, $c = \frac{\Gamma(y+\alpha)\Gamma(n+\beta-y)}{\Gamma(\alpha+\beta+n)}$. The expected value is

$$E(\theta|y) = \frac{y+\alpha}{n+\beta+\alpha} = \frac{n}{n+\beta+\alpha} \times \overbrace{\frac{y}{n}}^{\text{mle of }\theta} + \frac{\alpha+\beta}{n+\beta+\alpha} \times \frac{\alpha}{\alpha+\beta}.$$

The posterior mean is the weighted average of the mle $\widehat{\theta}$ and the prior mean as $n \to \infty$ converges to the mle. For $\alpha = \beta = 1$, we have the uniform distribution. $E(\theta|y) = \frac{y+1}{n+2}$, for the mle's $y = 0, \frac{1}{n+2}$, and for $y = n$, $\frac{n+1}{n+2}$ make more sense. The mle $\widehat{\theta} = \frac{y}{n}, 0 < \theta < 1$ *does not make sense.*

14.16 Rao-Cramer Inequality

Theorem: Let $\widehat{\theta}$ be an unbiased estimator of θ based on a random sample of size n from a distribution with the pdf $f(x|\theta)$. $Var(\widehat{\theta}) \geq \frac{1}{nI(\theta)}$ where

$$I(\theta) = E\left[\frac{d\log f}{d\theta}\right]^2 = -E\left[\frac{d^2\log f}{d\theta^2}\right].$$

This gives a lower bound for the variance used in the unbiased minimum variance estimators. It may not be achievable in some cases (such as the normal distribution). **Proof:** $T = \widehat{\theta} = T(x_1, x_2, ..., x_n)$, $L(\underline{x}|\theta) = \prod_{i=1}^n f(x_i|\theta)$.

1. $E(T) = \int TL(\underline{x}|\theta)d\underline{x} = \theta$.
2. $\int L(\underline{x}|\theta)d\underline{x} = 1$.

Recall the property that $\frac{dL}{d\theta} = \frac{1}{L}\frac{dL}{d\theta}L = \frac{d\log L}{d\theta}L$. Integrate (1) with respect to θ. Then,

$$0 = \int \frac{dL}{d\theta}d\underline{x} = \int \frac{d\log L}{d\theta}L(\underline{x}|\theta)d\underline{x} = E\left[\frac{d\log L}{d\theta}\right] = 0.$$

Call $z = \frac{d\log L}{d\theta}$, and $E(z) = 0$. Find $Cov(z,T) = E(Tz) - \overbrace{E(T)E(z)}^{=0}$. Integrate (1) with respect to θ.

$$1 = \int T \frac{dL}{d\theta} d\underline{x} = \int T \frac{d \log L}{d\theta} L(\underline{x}|\theta) d\underline{x} = E(Tz) = Cov(T, z) = 1.$$

$$\rho = Corr(T, z) = \frac{Cov(T, z)}{\sqrt{Var(T)Var(z)}}, \ \ \rho^2 = \frac{1}{Var(T)Var(z)} \leq 1 \Rightarrow Var(T) \geq \frac{1}{Var(z)} = nI(\theta).$$

Note that $z = \frac{d \log L}{d\theta} = \sum_{i=1}^{n} \frac{d \log f(x_i|\theta)}{d\theta}$ and

$$Var(z) = \sum_{i=1}^{n} Var\left(\frac{d \log f(x_i|\theta)}{d\theta}\right) = n \frac{d \log f(x|\theta)}{d\theta}.$$

$$\int f(x|\theta)\, dx = 1 \Rightarrow E\left(\frac{d \log f}{d\theta}\right) = 0.$$

Then,

$$Var\left[\frac{d \log f}{d\theta}\right] = E\left(\frac{d \log f}{d\theta}\right)^2,$$

$$\int \frac{d \log f}{d\theta} f(x|\theta)\, dx = 0.$$

Differentiate again.

$$\int \left[\frac{d^2 \log f}{d\theta^2} f(x|\theta) + \frac{d \log f}{d\theta}\frac{df}{d\theta}\right] dx = \int \frac{d^2 \log f}{d\theta^2} f(x|\theta)\, dx + \int \left(\frac{d \log f}{d\theta}\right)^2 f\, dx \Rightarrow E\left(\frac{d \log f}{d\theta}\right)^2 = -E\left(\frac{d^2 \log f}{d\theta^2}\right).$$

When does the equality hold here? $Var(\widehat{\theta}) \geq \frac{1}{nI(\theta)}$. When you want strict equality, $\rho^2 = 1$. This implies a linear relationship between z and T. $Corr(z, T-\theta) = Corr(z, T) = \pm 1$. $\frac{d \log L}{d\theta} = b(T-\theta)$. If $Corr(x, y) = \pm 1$, then $(y - \mu_x) = b(x - \mu_x)$. If $\exists$ a T unbiased for θ, such that $Var(T) = \frac{1}{nI(\theta)}$, then, how do we find that T? The mle of θ is found by solving $\frac{d \log L}{d\theta} = 0 \Rightarrow \widehat{\theta} = T$. So the mle will give the unbiased minimum variance estimator of θ achieving the Rao-Cramer lower bound if there exists such an estimator.

Example: $x \sim N(\mu, \theta)$. $\widetilde{\theta} = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$ is the biased mle. $\widehat{\theta} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$ is unbiased. Therefore, to achieve the lower bound on the variance, $\widetilde{\theta}$ must be the mle. Therefore, $\widetilde{\theta}$ cannot achieve the lower bound.

Corollary: If $\frac{d \log T}{d\theta} = b(T - \phi(\theta))$. Write, $\Phi(\theta) = \phi$ and T is the unbiased minimum variance estimator of Φ.

Corollary: If $E(T) = \Phi(\theta) = \theta + b(\theta)$ then T is a biased estimator of θ. $Var(T) \geq \frac{\Phi'(\theta)^2}{nI(\theta)} = \frac{(1+b'(\theta))^2}{nI(\theta)}$. **Proof:**

$$\int TL(\underline{x}|\theta) d\underline{x} = \Phi(\theta), \ \ Cov(T, z) = \Phi'(\theta).$$

So, $Corr(T, z) = \frac{\Phi'(\theta)}{\sqrt{Var(t)Var(z)}} = \rho$. $\rho^2 \leq 1$ implies the first equation.

Example: $x \sim Poisson(\theta)$.

$$L(\underline{x}|\theta) = \frac{e^{-n\theta}\theta^{\sum x_i}}{\prod x_i!}.$$

Call $\sum x_i = y$. Then, $\frac{d \log L}{d\theta} = -n + \frac{y}{\theta} = \frac{n}{\theta}\left(\frac{y}{n} - \theta\right) = \frac{n}{\theta}(T-\theta), T = \frac{y}{n}$ and $E(T) = 0$. T is the mle and unbiased for θ. $Var(T) = Var(\bar{x}) = \frac{\theta}{n}$. Also, $\frac{1}{nI(\theta)} = \frac{\theta}{n}$. Therefore, it is the unbiased minimum variance estimator because it achieves the lower bound.

14.17 Homework and Answers

These answers appear to be those of Siriluck's as the pages are Xeroxed and in her hand writing.

7.4 Let y_1 and y_2 be two independent unbiased estimators of θ. Say the variance of y_1 is twice the variance of y_2. Find the constants k_1 and k_2 so that $k_1y_1 + k_2y_2$ is an unbiased estimator with the smallest possible variance for such a linear combination.

y_1 and y_2 are two independent unbiased estimators of θ. Then, $E(y_1) = \theta, E(y_2) = \theta$. Define $Var(y_1) = 2Var(y_2)$. Consider $E(k_1y_1 + k_2y_2) = k_1E(y_1) + k_2k(y_2) = k_1\theta + k_2\theta = (k_1 + k_2)\theta$ and consider $Var(k_1y_1 + k_2y_2) = k_1^2 Var(y_1) + k_2^2 Var(y_2) = k_1^2 2Var(y_2) + k_2^2 Var(y_2) = (2k_1^2 + k_2^2)Var(y_2)$. From the first equation, k_1 and k_2 must be equal to 1 since we would like to have $k_1y_1 + k_2y_2$ to be an unbiased estimator of θ. Therefore $k_1 + k_2 = 1 \Rightarrow k_2 = 1 - k_1$. Consider $\frac{d}{dk_1}Var(k_1y_1 + k_2y_2) = \frac{d}{dk_1}[\{2k_1^2 + (1-k_1)^2\}Var(y_2)] = [4k_1 + 2(1-k_1)(-1)]Var(y_2) = 0 \Rightarrow 4k_1 - 2 + 2k_1 = 0 \Rightarrow k_1 = \frac{2}{6} = \frac{1}{3} \Rightarrow k_2 = 1 - \frac{1}{3} = \frac{2}{3}$. Check: $\frac{d^2}{dk_1^2}Var(k_1y_1 + k_2y_2) = 6 > 0 \Rightarrow$ it is the minimum. Therefore, $k_1 = \frac{1}{3}$ and $k_2 = \frac{2}{3}$ and $\frac{1}{3}y_1 + \frac{2}{3}y_2$ is an unbiased estimator with the smallest possible variance.

7.7 Let $x_1, x_2, ..., x_n$ denote a random sample from a distribution that is $N(\mu, \theta), 0 < \theta < \infty$ where μ is unknown. Let $y = \sum_{i=1}^n \frac{(x_i - \bar{x})^2}{n} = s^2$. And let $\text{Ł}[\theta, \delta(y)] = [\theta - \delta(y)]^2$. If we consider the decision functions of the form $\delta(y) = by$, where b does not depend upon y, show that $R(\theta, \delta) = (\theta^2/n^2)[(n^2-1)b^2 - 2n(n-1)b + n^2]$. Show that $b = \frac{n}{n+1}$ yields a minimum risk for the decision function of this form. Note that $\frac{ny}{n+1}$ is not an unbiased estimator of θ. With $\delta(y) = \frac{ny}{n+1}$ and $0 < \theta < \infty$, determine $\min R(\theta, \delta)$ if it exists. Consider

$$R(\theta, \delta) = E[\text{Ł}(\theta, \delta(y))] = E\{[\theta - \delta(y)]^2\} = E\{[\theta - by]^2\} =$$

$$E\{[\theta^2 - 2\theta by + b^2y^2]\} = E(\theta^2) - 2\theta bE(y) + b^2E(y^2) = \theta^2 - 2\theta b\frac{n-1}{n}\theta + b^2\left[\frac{2(n-1)\theta^2}{n^2} + \frac{(n-1)^2\theta^2}{n^2}\right].$$

From $y = s^2$, consider $\frac{ns^2}{\sigma^2} \sim \chi^2(n-1)$. In this case $\theta = \sigma^2$. $E(ns^2) = n-1$ and $Var\left(\frac{ns^2}{\sigma^2}\right) = 2(n-1)$. $E(y) = E(s^2) = \frac{(n-1)}{n}\theta$, and $Var(s^2) = \frac{2(n-1)\theta^2}{n^2}$. $E(y^2) = E(s^4) = Var(s^2) + [E(s^2)]^2 = \frac{2(n-1)}{n^2}\theta^2 + \frac{(n-1)^2}{n^2}\theta^2$. Getting back to the problem at hand, $R(\theta, \delta) = \frac{\theta^2}{n^2}\left[n^2 - 2n(n-1)b + 2(n-1)b^2 + (n-1)^2b^2\right] = \frac{\theta^2}{n^2}[n^2 - 2n(n-1)b + 2nb^2 - 2b^2 + n^2b^2 - 2nb^2 + b^2] = \frac{\theta^2}{n^2}[(n^2-1)b^2 - 2n(n-1)b + n^2]$. Consider $\frac{dR(\theta,\delta)}{db} = \frac{d}{db}\left[\frac{\theta^2}{n^2}\left\{(n^2-1)b^2 - 2n(n-1)b + n^2\right\}\right] = \frac{\theta^2}{n^2}\left\{2(n^2-1)b - 2n(n-1)\right\} = 0 \Rightarrow (n^2-1)b - 2n(n-1) = 0, \theta > 0$, $b = \frac{n(n-1)}{n^2-1} = \frac{n}{n+1}$. Check that it is the minimum. $\frac{d^2R(\theta,\delta)}{db^2} = \frac{\theta^2}{n}[2(n^2-1)b] \geq 0$. Therefore, $b = \frac{n}{n+1}$ yields a minimum risk for decision functions of this form. Consider $E\left[\frac{n}{n+1}y\right] = \frac{n}{n+1}E[y] = \frac{n}{n+1}\frac{n-1}{n}\theta = \frac{n-1}{n+1}\theta$. Therefore $\frac{ny}{n+1}$ is not an unbiased estimator of θ. Consider $R(\theta, \delta) = \frac{\theta^2}{n^2}[(n^2-1)b^2 - 2n(n-1)b + n^2]$ Here, $b = \frac{n}{n+1}$. Then, $R(\theta, \delta) = \frac{\theta^2}{n^2}\left[(n^2-1)\frac{n^2}{(n+1)^2} - 2n(n-1)\frac{n}{n+1} + n^2\right] = \frac{\theta^2}{n^2}\left[n^2\frac{(n-1)}{(n+1)} - 2\frac{n^2(n-1)}{(n+1)} + n^2\right] = \frac{\theta^2}{n^2}\left[n^2\frac{(n-1)}{(n+1)} + n^2\right] = \theta^2\left[\frac{n-1}{n+1} + 1\right] = \frac{2n\theta^2}{n+1}$. $\frac{d}{d\theta}R(\theta, \delta) = \frac{4n\theta}{n+1} = 0$. We can not find θ which gets $\min R(\theta, \delta)$. $\min_\theta R(\theta, \delta)$ does not exist.

7.8 Let $x_1, x_2, ..., x_n$ denote a random sample from a distribution that is $b(1,\theta), 0 \le \theta \le 1$. Let $y = \sum_{i=1}^{n} x_i$ and let $\text{Ł}[\theta, \delta(y)] = [\theta - \delta(y)]^2$. Consider the decision functions of the form $\delta(y) = by$, where b does not depend on y. Prove that $R(\theta,\delta) = b^2 n\theta(1-\theta) + (bn-1)^2\theta^2$. Show that $\max_\theta R(\theta,\delta) = \frac{b^4n^2}{4[b^2n-(bn-1)^2]}$, provided that the value of b is such that $b^2n \ge (bn-1)^2$. Prove that $b = \frac{1}{n}$ does not minimize $\max_\theta R(\theta,\delta)$. The pdf of x is

$$f(x|\theta) = \begin{cases} \theta(1-\theta)^x, & x = 0, 1; 0 \le \theta \le 1. \\ 0, & \text{otherwise.} \end{cases}$$

$y = \sum x_i \sim Binomial(n,\theta) \Rightarrow E(y) = n\theta; Var(y) = n\theta(1-\theta); \Rightarrow E(y^2) = Var(y) + [E(y)]^2 = n\theta(1-\theta) + n^2\theta^2$. Consider $R(\theta,\delta) = E[(\theta - by)^2] = E[\theta^2 - 2\theta by + b^2y^2] = \theta^2 - 2\theta bE(y) + b^2E(y^2) = \theta^2 - 2\theta b(n\theta) + b^2[n\theta(1-\theta) + n^2\theta^2] = \theta^2 - 2n\theta^2 b + b^2n\theta(1-\theta) + b^2n^2\theta^2 = b^2n\theta(1-\theta) + \theta^2 - 2n\theta^2 b + b^2n^2\theta^2 = b^2n\theta(1-\theta) + (1 - 2nb + b^2n^2)\theta^2 = b^2n\theta(1-\theta) + (bn-1)^2\theta^2$. Therefore, $R(\theta,\delta) = b^2n\theta(1-\theta) + (bn-1)^2\theta^2$. Now consider $\frac{d}{d\theta}R(\theta,\delta) = \frac{d}{d\theta}\left[b^2n\theta(1-\theta) + (bn-1)^2\theta^2\right] = b^2n - 2b^2n\theta + 2(bn-1)^2\theta = 0 \Rightarrow [2b^2n - 2(bn-1)^2]\theta = b^2n \Rightarrow \theta = \frac{b^2n}{[2b^2n-2(bn-1)^2]}$ Check that it is the maximum. $\frac{d^2}{d\theta^2}R(\theta,\delta) \ge 0$. $\max_\theta R(\theta,\delta) = b^2n\frac{b^2n}{2b^2n-2(bn-1)^2}\left(1 - \frac{b^2n}{2b^2n-2(bn-1)^2}\right) + (bn-1)^2\left(\frac{b^2n}{2b^2n-2(bn-1)^2}\right)^2 = \frac{b^4n^2}{2b^2n-2(bn-1)^2}\left[1 - \frac{b^2n}{2b^2n-2(bn-1)^2} + \frac{(bn-1)^2}{2b^2n-2(bn-1)^2}\right] = \frac{b^4n^2}{2b^2n-2(bn-1)^2}\left[\frac{2b^2n-2(bn-1)^2-b^2n+(bn-1)^2}{2b^2n-2(bn-1)^2}\right] = \frac{b^4n^2}{2b^2n-2(bn-1)^2}\left[\frac{b^2n-(bn-1)^2}{2b^2n-2(bn-1)^2}\right] = \frac{b^4n^2}{2b^2n-2(bn-1)^2}\left[\frac{1}{2}\left\{\frac{b^2n-(bn-1)^2}{b^2n-(bn-1)^2}\right\}\right] = \frac{b^4n^2}{4[b^2n-(bn-1)^2]}$. So, $\max_\theta R(\theta,\delta) = \frac{b^4n^2}{4[b^2n-(bn-1)^2]}$ provided that b is such that $b^2n \ge (bn-1)^2$. If this is true, then, $b^2n - b^2n^2 + 2bn - 1 \ge 0$, $-(n^2-n)b^2 + 2nb - 1 \ge 0 \Rightarrow b = \frac{-2n \pm \sqrt{4n^2 - 4(n^2-n)}}{-2(n^2-n)} = \frac{1}{n-1} \pm \frac{2\sqrt{n}}{2(n^2-n)} = \frac{1}{n-1} \pm \frac{\sqrt{n}}{n^2-n} = \frac{n \pm \sqrt{n}}{n^2-n}$. $b \ge \frac{n+\sqrt{n}}{n^2-n}$, or $b \le \frac{n-\sqrt{n}}{n^2-n}$. But, $b = \frac{1}{n}$ is in between $\left(\frac{n-\sqrt{n}}{n^2-n}, \frac{n+\sqrt{n}}{n^2-n}\right)$. So, b does not minimize $\max_\theta R(\theta,\delta)$.

7.17 What is the sufficient statistic for θ if the sample arises from a beta distribution in which $\alpha = \beta = \theta > 0$? $x \sim beta(\theta,\theta), \theta > 0$. The pdf is $f(x) = \frac{\Gamma(2\theta)}{(\Gamma(\theta))^2}x^{\theta-1}(1-x)^{\theta-1}, 0 < x < 1$. Consider

$$\prod_{i=1}^{n} f(x_i|\theta) = \prod_{i=1}^{n} \frac{\Gamma(2\theta)}{(\Gamma(\theta))^2} x_i^{\theta-1}(1-x_i)^{\theta-1} = \frac{(\Gamma(2\theta))^n}{(\Gamma(\theta))^{2n}} \prod_{i=1}^{n}[x_i(1-x_i)]^{\theta-1} = k_1[\prod_{i=1}^{n} x_i(1-x_i), \theta]k_2\underline{x},$$

where $k_2\underline{x} = 1$. By using the Factorization Theorem, $T = \prod_{i=1}^{n} x_i(1-x_i)$ is the sufficient statistic for θ.

7.20 If x_1, and x_2 is a random sample of size 2 from the distribution have the pdf $f(x,\theta) = \frac{1}{\theta}e^{-x/\theta}, 0 < x < \infty, 0 < \theta < \infty$, and zero otherwise, find the joint pdf of the sufficient statistic $y_1 = x_1 + x_2$ for θ and $y_2 = x_2$. Show that y_2 is an unbiased estimator of θ with the variance θ^2. Find $E[y_2|y_1] = \phi(y_1)$ and the variance of $\phi(y_1)$. We can find the joint pdf of $y_1 = x_1 + x_2$ by using the formulation on page 178 of the text book.

$$g(y_1, y_2) = f_1(y_1 - y_2)f_2(y_2) = \frac{1}{\theta}e^{-\frac{y_1-y_2}{\theta}} \times \frac{1}{\theta}e^{-y_2/\theta} = \frac{1}{\theta^2}e^{-y_1/\theta}.$$

Then, the joint pdf of y_1 and y_2 is

$$g(y_1, y_2) = \begin{cases} \frac{1}{\theta^2}e^{-y_1/\theta}, & 0 < y_2 < y_1 < \infty. \\ 0, & \text{otherwise.} \end{cases}$$

Therefore, $y_2 = x_2$ implies that the pdf of y_2 is

$$g_2(y_2) = \begin{cases} \frac{1}{\theta}e^{-y_2/\theta}, & 0 < y_2 < \infty. \\ 0, & \text{otherwise.} \end{cases}$$

Consider

$$E(y_2) = \int_0^\infty y_2 \frac{1}{\theta} e^{-y_2/\theta}\, dy_2 = \Gamma(2)\theta \int_0^\infty \frac{1}{\Gamma(2)\theta^2} y_2^{2-1} e^{-y_2/\theta}\, dy_2 = \theta$$

because

$$\Gamma(2) \int_0^\infty \frac{1}{\Gamma(2)\theta^2} y_2^{2-1} e^{-y_2/\theta}\, dy_2 = 1$$

since it is $Gamma(2, \theta)$. Therefore, y_2 is an unbiased estimator for θ. Consider,

$$E(y_2^2) = \int_0^\infty y_2^2 \frac{1}{\theta} e^{-y_2/\theta}\, dy_2 = \Gamma(3)\theta^2 \int_0^\infty \frac{1}{\Gamma(3)\theta^3} y_2^{3-1} e^{-y_2/\theta}\, dy_2 = 2\theta^2.$$

Hence, $Var(y_2) = E(y_2^2) - [E(y_2)]^2 = 2\theta^2 - \theta^2 = \theta^2$. Hence, y_2 is an unbiased estimator for θ with a variance of θ^2. From the convolution formula on page 178 of the text book,

$$g_1(y_1) = \int_{-\infty}^\infty f_1(y_1 - y_2) f_2(y_2)\, dy_2 = \int_{-\infty}^\infty g(y_1, y_2)\, dy_2 =$$

$$\int_0^{y_1} \frac{1}{\theta^2} e^{-y_1/\theta}\, dy_2 = \begin{cases} \frac{1}{\theta^2} e^{-y_1/\theta} y_1, & 0 < y_1 < \infty. \\ 0, & \text{otherwise.} \end{cases}$$

The conditional pdf of y_2 given y_1 is

$$g(y_2|y_1) = \frac{g(y_1, y_2)}{g_1(y_1)} = \frac{\frac{1}{\theta^2} e^{-y_1/\theta}}{\frac{1}{\theta^2} e^{-y_1/\theta} y_1} = \frac{1}{y_1}, 0 < y_2 < y_1.$$

Therefore the expected value

$$E(y_2|y_1) = \int_0^{y_1} y_2 \frac{1}{y_1}\, dy_2 = \frac{1}{y_1} \frac{y_2^2}{2}\Big|_0^{y_1} = \frac{y_1}{2}, 0 < y_1 < \infty.$$

Therefore, $E(y_2|y_1) = \frac{y_1}{2} = \phi(y_1)$. Since $y_1 \sim Gamma(2, \theta)$, $Var(\phi(y_1)) = Var\left(\frac{y_1}{2}\right) = \frac{1}{4} Var(y_1) = \frac{1}{4} 2\theta^2 = \frac{\theta^2}{2}$.

7.25 Let $x_1, x_2, ..., x_n$ represent a random sample from the discrete distribution having the probability density function

$$f(x, \theta) = \begin{cases} \theta^x (1-\theta)^{1-x}, & x = 0, 1, 0 < \theta < 1. \\ 0, & \text{otherwise.} \end{cases}$$

Show that $y = \sum_{i=1}^n x_i$ is a complete sufficient statistic for θ. Find the unique function of y_1, that is the unbiased minimum variance estimator of θ. Hint: Show that $E[u(y_1)] = 0$ and that the constant term $u(0) = 0$, divide both members of the equation by $\theta \neq 0$, and repeat the argument.

It is given that $x \sim Bernoulli(\theta)$.

$$\prod_{i=1}^{n} f(x_i|\theta) = \prod_{i=1}^{n} \theta^{x_i}(1-\theta)^{1-x_i} = \theta^{\sum x_i}(1-\theta)^{n-\sum x_i} = k_1\left(\sum x_i, \theta\right) k_2(\underline{x}).$$

By using the Factorization Theorem, $\sum x_i$ is sufficient for θ. Let $y = \sum x_i$. We know that $y \sim binomial(n, \theta)$. Consider

$$E(u(y)) = 0, \forall\theta, \sum_{y=0}^{\infty} u(y) \begin{pmatrix} n \\ y \end{pmatrix} \theta^y (1-\theta)^{n-y} = 0, \forall\theta, \sum_{y=0}^{\infty} u(y) \begin{pmatrix} n \\ y \end{pmatrix} \left(\frac{\theta}{1-\theta}\right)^y = 0$$

We compare the coefficient of

$$\left(\frac{\theta}{1-\theta}\right)^y, \quad u(y) \begin{pmatrix} n \\ y \end{pmatrix} = 0, \forall y, \Rightarrow u(y) = 0, \forall y$$

and conclude that $g(y|\theta)$ is a complete family. From the two conclusions given so far, we can conclude that $y = \sum_{i=1}^{n} x_i$ is a complete sufficient statistic for θ. Consider

$$E(y) = E\left(\sum_{i=1}^{n} x_i\right) = n\theta \Rightarrow E\left(\frac{y}{n}\right) = \theta.$$

Therefore, $\frac{y}{n}$ is an unbiased estimator for θ. From the three conclusions given so far, we can conclude that $\frac{y}{n}$ is the unique function of y_1 that is the unbiased minimum variance estimator for θ.

7.27 Show that the first order statistic y_1 of a random sample of size n from the distribution having the pdf $f(x, \theta) = e^{-(x-\theta)}, \theta < x < \infty, -\infty < \theta < \infty$ and zero elsewhere, is a complete sufficient statistic for θ. Find the unique function of this statistic which is the unbiased minimum variance estimator of θ. The cdf of x is

$$F(x) = \int_{\theta}^{x} e^{-(u-\theta)} du = -e^{-(u-\theta)}\Big|_{\theta}^{x} = 1 - e^{-(x-\theta)}.$$

Therefore the cdf is given by

$$F(x) = \begin{cases} 0, & x \leq \theta. \\ 1 - e^{-(x-\theta)}, & x > \theta. \end{cases}$$

We can find the pdf of y_1 from this formula.

$$g_1(y_1) = \begin{cases} n[1 - F(y_1)]^{n-1} f(y_1), & a < y_1 < b. \\ 0, & \text{otherwise.} \end{cases}$$

$$g_1(y_1|\theta) = \begin{cases} n[1 - (1 - e^{-(y_1-\theta)})]^{n-1} e^{-(y_1-\theta)}, & \theta < y_1 < \infty. \\ 0, & \text{otherwise.} \end{cases}$$

Consider $E[u(y_1)] = 0 \,\forall\theta$,

$$\int_\theta^\infty u(y_1) g_1(y_1|\theta)\, dy_1 = 0, \; \int_\theta^\infty u(y_1) n e^{-n(y_1-\theta)}\, dy_1 = 0, \; \int_\theta^\infty u(y_1) e^{-n(y_1-\theta)}\, dy_1 = 0,$$

(by dividing both sides by n). Next integrate by parts. Let $v = y_1 - \theta$, and $dv = dy_1$. If $y_1 = \theta$, then $v = 0$, and if $y_1 = \infty$, the $v = \infty$. Therefore we have

$$\int_0^\infty u(y_1) e^{-nv} dv = 0.$$

The Laplace transform is

$$\int_0^\infty u(y_1) e^{-tv} dv = 0.$$

Then, $u(y_1) = 0, \forall y_1 > \theta \Rightarrow u(v + \theta) = 0, \forall v + \theta \Rightarrow u(y_1) = 0, \forall y_1$. Therefore, $g_1(y_1|\theta)$ is a complete family. Consider the joint distribution of $x_1, x_2, ..., x_n$.

$$\prod_{i=1}^n f(x_i|\theta) = \prod_{i=1}^n e^{-(x_i-\theta)} = e^{-\sum x_i + n\theta}, \theta < x_i < \infty, -\infty < \theta < \infty.$$

Notice that the range depends on θ. So, we will write the pdf in the following form. $\prod_{i=1}^n f(x_i|\theta) = e^{-\sum x_i + n\theta} I_A(x_{(1)}), -\infty < x_i < \infty, i = 1, 2, ..., n$. Then, $(\sum x_i, x_{(1)})$ are jointly sufficient for θ and $x_{(1)} = y_1$. Thus, y_1 is a sufficient statistic for θ. From these results, we can conclude that y_1 is a complete sufficient statistic for θ.

Consider

$$E(y_1) = \int_\theta^\infty y_1 g_1(y_1|\theta)\, dy_1 = \int_\theta^\infty y_1 n e^{-n(y_1-\theta)}\, dy_1 = e^{n\theta} n \int_\theta^\infty y_1 e^{-ny_1}\, dy_1 =$$

$$ne^{n\theta} \left[\frac{e^{-ny_1}}{-n} \left(y_1 - \frac{1}{-n} \right) \right]_\theta^\infty = \theta + \frac{1}{n} \Rightarrow E\left(y_1 - \frac{1}{n} \right) = \theta.$$

Therefore, $\psi(y_1) = y_1 - \frac{1}{n}$ is an unbiased estimator for θ. Therefore, y_1 is a sufficient statistic for θ, and $g_1(y_1|\theta)$ is a complete family. Also, $\psi(y_1)$ is an unbiased estimator for θ and $\psi(y_1) = y_1 - \frac{1}{n}$ is a unique function of y_1 which is the unbiased minimum variance estimator of θ.

7.42 In the notation of Example 2 in the text book of Section 7, is there an unbiased minimum variance estimator of $P(-r \le x \le r)$? Let $\phi(\theta) = P(-r \le x \le r)$, where $r > 0$. Then,

$$\phi(\theta) = \int_{-r}^{r} \frac{e^{-\frac{(x-\theta)^2}{2}}}{\sqrt{2\pi}}\, dx$$

and we know that $\bar{x}$ is a complete sufficient statistic for θ. $x_1, x_2, ..., x_n$ is the random sample. Consider

$$u(x_1) = \begin{cases} 1, & \text{if } -r \le x_1 \le r. \\ 0, & \text{otherwise.} \end{cases}$$

The expected value is

$$E[u(x_1)] = 1P(-r \le x_1 \le r) + 0P(-r \le x_1 \le r) = \phi(\theta),\ \ x_1|\bar{x} \sim N\left(\bar{x}, \frac{n-1}{n}\right).$$

$$\psi(\bar{x}) = E[u(x_1)|\bar{x}] = P(-r \le x_1 \le r|\bar{x}) = \int_{-r}^{r} \frac{e^{-\frac{(x_1-\bar{x})^2 n}{2(n-1)}}}{\sqrt{2\pi\frac{n-1}{n}}}\, dx_1 =$$

$$\int_{-\infty}^{(r-\bar{x})\sqrt{\frac{n}{n-1}}} \frac{e^{-\frac{z^2}{2}}}{\sqrt{2\pi}}\, dz - \int_{-\infty}^{(-r-\bar{x})\sqrt{\frac{n}{n-1}}} \frac{e^{-\frac{z^2}{2}}}{\sqrt{2\pi}}\, dz = \Phi\left((r-\bar{x})\sqrt{\frac{n}{n-1}}\right) - \Phi\left((-r-\bar{x})\sqrt{\frac{n}{n-1}}\right).$$

There is a minimum unbiased variance estimator and it is $\Phi\left((r-\bar{x})\sqrt{\frac{n}{n-1}}\right) - \Phi\left((-r-\bar{x})\sqrt{\frac{n}{n-1}}\right)$.

7.46 Let $y_1 < y_2 < y_3$ be the order statistics of a random sample of size 3 from the distribution

$$f(x, \theta_1, \theta_2) = \begin{cases} \frac{1}{\theta_2} e^{-\frac{x-\theta_1}{\theta_2}}, & \theta_1 < x < \infty, -\infty < \theta_1 < \infty, 0 < \theta_2 < \infty. \\ 0, & \text{otherwise.} \end{cases}$$

Find the joint pdf of $z_1 = y_1, z_2 = y_2$, and $z_3 = y_1 + y_2 + y_3$. The corresponding transformation maps the space $\{(y_1, y_2, y_3) : \theta_1 < y_1 < y_2 < y_3 < \infty\}$ onto $\{(z_1, z_2, z_3) : \theta_1 < z_1 < z_2 < \frac{(z_3-z_1)}{2} < \infty\}$. Show that z_1 and z_3 are joint sufficient statistics for θ_1 and θ_2.

The joint pdf if y_1, y_2 and y_3 is

$$f(y_1, y_2, y_3; \theta_1, \theta_2) =$$

$$3!\prod_{i=1}^{3} g(y_i; \theta_1, \theta_2), \theta_1 < y_1 < y_2 < y_3 < \infty = \begin{cases} \frac{6}{\theta_2^3} e^{-\frac{(y_1+y_2+y_3)}{\theta_2} - 3\frac{\theta_1}{\theta_2}}, & \theta_1 < y_1 < y_2 < y_3 < \infty. \\ 0, & \text{otherwise.} \end{cases}$$

Let $z_1 = y_1, z_2 = y_2$ and $z_3 = y_1 + y_2 + y_3$. Then, $y_1 = z_1, y_2 = z_2$, and $y_3 = z_3 - z_1 - z_2$. The Jacobian matrix is

$$J = \begin{vmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{vmatrix} = 1$$

Thus, the joint pdf of z_1, z_2, and z_3 is $h(z_1, z_2, z_3; \theta_1, \theta_2) = g(z_1, z_2, z_3 - z_2 - z_1)|J| = \frac{6}{\theta_2^3} e^{-\frac{z_3}{\theta_2} - \frac{3\theta_1}{\theta_2}} \times 1, \theta_1 < z_1 < z_2 < \frac{z_3 - z_1}{2} < \infty = \frac{6}{\theta_2^3} e^{-\frac{z_3}{\theta_2} - \frac{3\theta_1}{\theta_2}} I_A((\theta_1), -\infty < z_1 < z_2 < \frac{z_3 - z_1}{2} < \infty$. Therefore, (z_1, z_3) are joint sufficient statistics for θ_1 and θ_2 since the range depends on θ_1 from z_1, and z_3 depends on θ_2.

7.54 Let $y_1 < y_2 < \cdots < y_n$ be the order statistics of a random sample of size n from the uniform distribution over the closed interval $[-\theta, \theta]$ having the pdf $f(x; \theta) = \frac{1}{2\theta} I_{[-\theta, \theta]}(x)$

a. Show that y_1 and y_n are joint sufficient statistics for θ.

The joint pdf of $y_1, y_2, ..., y_n$ is

$$g(y_1, y_2, ..., y_n; \theta) = n! \prod_{i=1}^{n} f(y_i), -\theta \le y_1 < y_2 < \cdots < y_n \le \theta =$$

$$\frac{n!}{(2\theta)^n} \prod_{i=1}^{n} I_{[-\theta, \theta]}(y_i) = \frac{n!}{(2\theta)^n} I_A(y_1, y_n), -\infty < y_1 < y_2 < \cdots < y_n < \infty.$$

I_A is such that $A : \{-\theta \le y_1 < y_n \le \theta\}$. From the Factorization Theorem, we can conclude that (y_1, y_n) are joint sufficient statistics for θ.

b. Argue that the mle of θ equals $\widehat{\theta} = \max(-y_1, y_n)$.

$$L(\theta|\underline{x}) = \prod_{i=1}^{n} \frac{1}{2\theta} = \frac{1}{(2\theta)^n}, -\theta < x_i < \theta.$$

L is a decreasing function as θ increases. Let $y_1 < y_2 < \cdots < y_n$ be the ordered sample. Then, $-\theta < y_1 < y_2 < \cdots < y_n \le \theta$. Therefore $\theta \ge y_n$ or $-\theta \le y_1 \Rightarrow \theta \le -y_1$. Therefore, $\widehat{\theta} = \max(-y_1, y_n)$. Therefore it must be the mle.

c. Demonstrate that the mle $\widehat{\theta}$ is a sufficient statistic for θ and thus is a minimum sufficient statistic for θ.

$$f(\theta|\underline{y}) = \frac{n!}{(2\theta)^n} I_A(y_1, y_n) \times 1$$

which gives us $k_1(f, \theta)$ and $k_2(y) = 1$ does not depend on θ. $\widehat{\theta} = \max(-y_1, y_n)$ is a function of y_1 and y_n. Therefore the mle $\widehat{\theta}$ is a sufficient statistic for θ and thus is a minimal sufficient statistic for θ. See Figure 14.11.

Additional Problem: $E|x - \theta|$ is the minimum if $\theta = median(x)$. For this problem, recall the calculus property of integration when θ is both part of the upper and lower bounds and part of the integrand.

$$\frac{d}{d\theta} \int_{a(\theta)}^{b(\theta)} f(x)\, dx = \frac{db}{d\theta} f(b(\theta)) - \frac{da}{d\theta} f(a(\theta)).$$

Then, to solve the problem at hand.

$$A(\theta) = E|x - \theta| = \int_{-\infty}^{\infty} |x - \theta| f(x)\, dx = \int_{-\infty}^{\theta} |x - \theta| f(x)\, dx + \int_{\theta}^{\infty} |x - \theta| f(x)\, dx =$$

$$\int_{-\infty}^{\theta} (\theta - x) f(x)\, dx + \int_{\theta}^{\infty} (x - \theta) f(x)\, dx = \theta F(\theta) - \int_{-\infty}^{\theta} x f(x)\, dx + \int_{\theta}^{\infty} x f(x)\, dx - \theta[1 - F(\theta)].$$

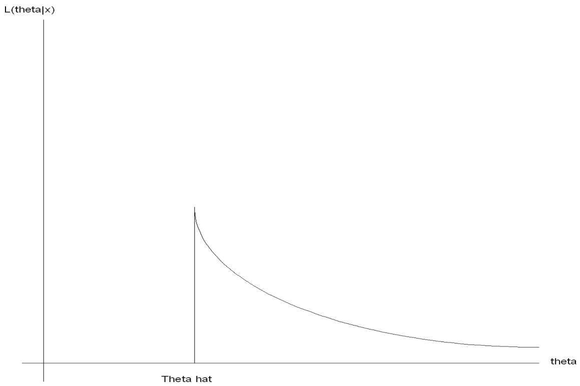

Figure 14.11: This figure shows the shape of the curve for the mle $\widehat{\theta} = \max(-y_1, y_n)$.

$$A(\theta) = 2\theta F(\theta) - \theta - \int_{-\infty}^{\theta} x f(x)\, dx + \int_{\theta}^{\infty} x f(x)\ dx,$$

$$\frac{dA}{d\theta} = 2[F(\theta) + \theta f(\theta)] - 1 - \theta f(\theta) - \theta f(\theta) = 2F(\theta) - 1 = 0 \Rightarrow F(\theta) = \frac{1}{2} \Rightarrow \theta = median(x).$$

Additional Problem: $\widehat{\mu} = \sum_{i=1}^{n} a_i x_i + b,\ E(\widehat{\mu}) = \sum_{i=1}^{n} a_i E(x_i) + b = \mu \sum_{i=1}^{n} a_i + b = \mu$ want to be unbiased $\forall \mu$. Therefore, the following two must be true. $b = 0$ and $\sum_{i=1}^{n} a_i = 1$. Now, $\widehat{\mu} = \sum_{i=1}^{n} a_i x_i$, and $Var(\widehat{\mu}) = \sigma^2 \sum_{i=1}^{n} a_i^2$. Minimize $\sum_{i=1}^{n} a_i^2$ subject to $\sum_{i=1}^{n} a_i = 1$. Another way to minimize this is to set the following equation up.

$$\sum_{i=1}^{n-1} a_i^2 + (1 - a_1 - a_2 - \cdots - a_{n-1})^2 = A$$

$$\frac{d\,A}{d\,a_i} = 2a_i - 2(1 - a_1 - a_2 - \cdots - a_{n-1}), i = 1, 2, ..., n-1.$$

$$a_i = (1 - a_1 - a_2 - \cdots - a_{n-1}), i = 1, 2, ..., n-1.$$

$$a_i = a_n, i = 1, 2, ..., n-1. \Rightarrow a_i = a, \forall i.$$

Since $\sum_{i=1}^{n} a_i = 1 \Rightarrow a = \frac{1}{n}$.

14.18 More on the Rao-Cramer Lower Bound

If $\widehat{\theta}$ is unbiased for θ, then $Var(\widehat{\theta}) = \frac{1}{nI(\theta)}$. If T is an unbiased estimator for θ, the *efficiency* of T is

$$E = \frac{\text{Lower Bound}}{Var(T)} = \frac{\frac{1}{nI(\theta)}}{Var(T)}.$$

For the multi parameter case, $\theta' = (\theta_1, \theta_2, ..., \theta_k)$.

$$-E\left[\frac{d^2 \log f}{d\theta_i d\theta_j}\right] = E\left[\frac{d \log f}{d\theta_i} \frac{d \log f}{d\theta_j}\right] = I_{ij}.$$

I_{ij} is called the *information matrix.* $I(\theta) = (I_{ij})_{k\times k}$. Let $T' = (T_1, T_2, ..., T_k)$ be unbiased for θ'. $E(T) = \theta$. The covariance matrix is $\not{\sum}_T = \{E(T_i - \theta_i)(T_j - \theta_j)\}_{k\times k}$.

Theorem: $\not{\sum}_T - \frac{1}{n} I^{-1}(\theta)$ is a positive semi-definite matrix.

$$Var(T_i) \geq \frac{\overbrace{I^{ii}(\theta)}^{\text{diagonal}}}{n} \text{ where } I^{-1}(\theta) = \{I^{ij}\}_{k\times k}.$$

Example: $x \sim N(\theta_1, \theta_2)$.

$$f(x|\theta) = \frac{1}{\sqrt{2\pi\theta_2}} e^{-\frac{(x-\theta_1)^2}{2\theta_2}}, \ \log f = c - \frac{1}{2}\log\theta_2 - \frac{1}{2\theta_2}(x-\theta_1)^2.$$

We know that $T_1 = \bar{x}$ and $T_2 = S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$.

$$T = \begin{pmatrix} T_1 \\ T_2 \end{pmatrix} \text{ is unbiased for } \theta = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix}.$$

$$\frac{(n-1)T_2}{\theta_2} \sim \chi^2(n-1).$$

$$Var\left[\frac{(n-1)T_2}{\theta_2}\right] = 2(n-1), \ Var(T_2) = \frac{2\theta_2^2}{n-1}.$$

$$\not{\sum}_T = \begin{pmatrix} \frac{\theta_2}{T} & 0 \\ 0 & \frac{2\theta_2^2}{n-1} \end{pmatrix}.$$

$$\frac{d\log f}{d\theta_1} = \frac{x-\theta_1}{\theta_2}, \ \frac{d^2\log f}{d\theta_1^2} = -\frac{1}{\theta_2}, \ \frac{d^2\log f}{d\theta_2\theta_1} = -\frac{(x-\theta_1)}{\theta_2^2}$$

$$\frac{d\log f}{d\theta_2} = -\frac{1}{2\theta_2} + \frac{(x-\theta_1)^2}{2\theta_1^2}, \ \frac{d^2\log f}{d\theta_2^2} = \frac{1}{2\theta_2^2} - \frac{(x-\theta_1)^2}{\theta_2^3}.$$

$$I(\theta) = \begin{pmatrix} \frac{1}{\theta_2} & 0 \\ 0 & \frac{1}{2\theta_2^2} \end{pmatrix}, \ -E\left[\frac{d\log f}{d\theta_2^2}\right] = -\frac{1}{2\theta_2^2} + \frac{1}{\theta_2^2} = \frac{1}{2\theta_2^2}.$$

$$\frac{1}{n}I^{-1}(\theta) = \begin{pmatrix} \frac{\theta_2}{n} & 0 \\ 0 & \frac{2\theta_2^2}{n} \end{pmatrix} = \not{\sum}_T$$

which implies that the lower bound is not achieved. But, $Var(S^2) > \frac{2\theta_2^2}{n}$ is still the unbiased minimum variance estimator even though the lower bound is not achieved.

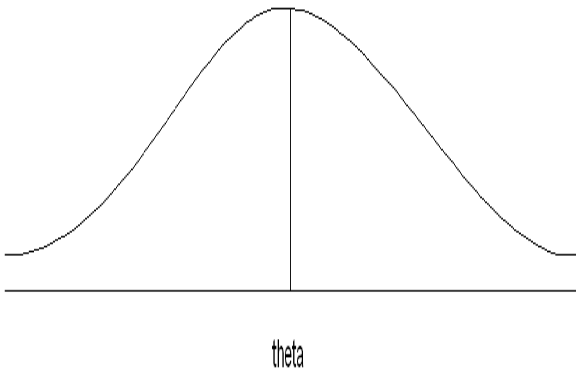

Figure 14.12: The Chaucy distribution is symmetric about θ.

14.19 The Cauchy Distribution

Homework 3: Chapter 8, problems 8.2, 8.15, 8.19, 8.28. Chapter 9, problems 9.10, 9.12, 9.22, 9.30, 9.37, 9.39. Also, solve the following problem: Let x have the pdf $f(x|\theta), -\infty < x < \infty$. If $\widehat{\theta}$ is an estimator of θ with $E(\widehat{\theta}) = \theta + b(\theta)$, then prove that $Var(\widehat{\theta}) \geq \frac{(1+b'(\theta))^2}{nI(\theta)}$.

The Cauchy distribution has the following pdf. See also Figure 14.12.

$$f(x|\theta) = \left\{ \frac{1}{\pi[1+(x-\theta)^2]}, \quad -\infty < x < \infty. \right.$$

The expected value $E(x)$ does not exist because

$$E(x) = \int_{-\infty}^{\infty} \frac{x}{\pi[1+(x-\theta)^2]}\,dx,$$

Let $x - \theta = y$. Then, we have

$$\int_{-\infty}^{\infty} \frac{y+\theta}{\pi[1+y^2]}\,dy = \int_{-\infty}^{\infty} \frac{1}{\pi}\frac{y}{1+y^2}\,dy + \theta\int_{-\infty}^{\infty} \frac{1}{\pi(1+y^2)}\,dy.$$

Note that

$$\int_{-\infty}^{0} \frac{y}{\pi(1+y^2)}\,dy + \theta\overbrace{\int_{0}^{\infty} \frac{y}{\pi(1+y^2)}\,dy}^{\text{not finite}}.$$

We must show that $E|x|$ exists for $E(x)$ to exist. Let θ be the median of x. Then, $P(x<\theta) = P(x>\theta) = \frac{1}{2}$. To estimate $\theta, \bar{x}$ has the same distribution as that of x which is useless. A characteristic function where i is a *complex variable*, $e^{ia} = \cos a + i\sin a$

$$\phi_x(t) = E[e^{itx}], |e^{itx}| \leq 1, \;\; E[e^{itx}] = e^{-|t|}e^{t\theta},$$

$$\phi_{\bar{x}}(t) = E[e^{itx}] = E\left[\prod_{i=1}^{n} e^{i\frac{t}{n}x_i}\right] = \prod_{i=1}^{n} E\left[e^{i\frac{t}{n}x_i}\right] = \prod_{i=1}^{n}\left[e^{-|\frac{t}{n}|}e^{\frac{t}{n}\theta}\right] = e^{-|t|}e^{t\theta}.$$

The mle is

$$\log L = c - \sum_{i=1}^{n} \log[1+(x_i-\theta)^2], \quad \frac{d\log L}{d\theta} = 2\sum_{i=1}^{n} \frac{x_i-\theta}{1+(x_i-\theta)^2} = 0.$$

The equation can be solved numerically. Let's say m is the sample median. $\widehat{\theta} = m$. Asymptotically though, it is not fully efficient. $Var(\widehat{\theta}) \geq \frac{1}{nI(\theta)}$ The asymptotic variance of m is $Var(m) = \frac{\pi^2}{4n} > \frac{1}{nI(\theta)}$.

14.20 Asymptotic Distribution of the MLE $\widehat{\theta}$

$$L(\theta|\underline{x}) = \prod_{i=1}^{n} f(x_i|\theta), \ \ \log L = \sum_{i=1}^{n} \log f(x_i|\theta), \ \ z = \frac{d\log L}{d\theta} = \sum_{i=1}^{n} \frac{d\log f(x_i|\theta)}{d\theta} = \sum_{i=1}^{n} y_i$$

where $y_1, y_2, ..., y_n$ are iid. Then, z has a normal distribution.

$$E(z) = E\left[\frac{d\log L}{d\theta}\right] = 0, \ \ Var(z) = nI(\theta),$$

where

$$I(\theta) = E\left[\frac{d\log f}{d\theta}\right]^2 = -E\left[\frac{d^2\log f}{d\theta^2}\right], \quad \frac{z-0}{\sqrt{nI(\theta)}} = \frac{(\bar{y}-0)\sqrt{n}}{\sqrt{I(\theta)}} \to N(0,1).$$

$\widehat{\theta}$ is such that $\left(\frac{d\log L}{d\theta}\right)_{\theta=\widehat{\theta}} = 0 = \frac{d\log L}{d\widehat{\theta}}$. Using Taylor's series expansion,

$$0 = \frac{d\log L}{d\widehat{\theta}} = \frac{d\log L}{d\theta} + (\widehat{\theta}-\theta)\frac{d^2\log L}{d\theta^2} + (\widehat{\theta}-\theta)^2 \overbrace{\left(\frac{d^3\log L}{d\theta^3}\right)_{\theta^*}}^{\text{Error Term}} - (\widehat{\theta}-\theta)\frac{d^2\log L}{d\theta^2} =$$

$$\frac{d\log L}{d\theta} + (\widehat{\theta}-\theta)^2\left(\frac{d^3\log L}{d\theta^3}\right)_{\theta^*} - \sqrt{n}(\widehat{\theta}-\theta)\frac{d^2\log L}{d\theta^2} = \frac{\sqrt{n}d\log L}{d\theta} + \sqrt{n}(\widehat{\theta}-\theta)^2\left(\frac{d^3\log L}{d\theta^3}\right)_{\theta^*}$$

It is known that $(\widehat{\theta}-\theta) \xrightarrow{P} 0$. We need to find the distribution of $\sqrt{n}(\widehat{\theta}-\theta)$.

$$\overbrace{\sqrt{n}(\widehat{\theta}-\theta)}^{\text{random}}\overbrace{(\widehat{\theta}-\theta)}^{\to 0}\frac{d^3\log L}{d\theta^3} \to 0.$$

If $x_n \xrightarrow{D} x$, $y_n \xrightarrow{P} c$, then $x_n y_n \xrightarrow{D} x_c^*$.

$$\sqrt{n}(\widehat{\theta}-\theta) = -\sqrt{n}\frac{\frac{d\log L}{d\theta}}{\left(\frac{d^2\log L}{d\theta^2}\right)} = \frac{z\sqrt{n}}{\left(-\frac{d^2\log L}{d\theta^2}\right)}, \quad -\frac{d^2\log L}{nd\theta^2} = \frac{1}{n}\sum_{i=1}^{n} -d^2\frac{\log f(x_i|\theta)}{d\theta^2} \xrightarrow{P} -E\left[d^2\frac{\log f(x_i|\theta)}{d\theta^2}\right] = I(\theta).$$

Then,

$$(\widehat{\theta}-\theta) = -\frac{\frac{d\log L}{d\theta}}{\frac{d^2\log L}{d\theta^2}} = \frac{z}{-\frac{d^2\log L}{d\theta^2}} = \frac{z}{\sqrt{nI(\theta)}}\left(\frac{\sqrt{nI(\theta)}}{-\frac{d^2\log L}{d\theta^2}}\right).$$

Then,

$$\sqrt{n}(\widehat{\theta}-\theta) = \frac{z}{\sqrt{nI(\theta)}}\left(\frac{n\sqrt{I(\theta)}}{-\frac{d^2\log L}{d\theta^2}}\right), \quad \frac{n\sqrt{I(\theta)}}{-\frac{d^2\log L}{d\theta^2}} = \frac{\sqrt{I(\theta)}}{-\frac{1}{n}\frac{d^2\log L}{d\theta^2}} \xrightarrow{P} \frac{\sqrt{I(\theta)}}{I(\theta)} = \frac{1}{\sqrt{I(\theta)}}.$$

Then, the whole thing converges to

$$\frac{z}{\sqrt{nI(\theta)}}\frac{n\sqrt{I(\theta)}}{-\frac{d^2\log L}{d\theta^2}} \xrightarrow{D} U\frac{1}{\sqrt{I(\theta)}} \Rightarrow \sqrt{n}(\widehat{\theta}-\theta)\sqrt{I(\theta)} \to U \sim N(0,1).$$

This is the same thing as saying that $\sqrt{n}(\widehat{\theta}-\theta) \to N\left(0, \frac{1}{I(\theta)}\right)$. The asymptotic result is $(\widehat{\theta}-\theta) \to N\left(0, \frac{1}{nI(\theta)}\right)$. The variance is the lower bound. Thus, the mle achieves the Rao-Cramer lower bound for large n.

Example: $f(x|\theta) = \theta x^{\theta-1}, 0 < x < 1$. The mle of θ is

$$\widehat{\theta} = \frac{-n}{\log\prod_{i=1}^n x_i}.$$

The exact distribution of $\widehat{\theta}$ can not be found in a closed form. Recall that $\sqrt{n}(\widehat{\theta}-\theta) \to N\left(0, \frac{1}{I(\theta)}\right)$ where $I(\theta)$ is found by $\frac{d\log f}{d\theta} = \frac{1}{\theta} + \log x$, $-\frac{d^2\log f}{d\theta^2} = \frac{1}{\theta^2} \Rightarrow I(\theta) = \frac{1}{\theta^2} \Rightarrow \sqrt{n}(\widehat{\theta}-\theta) \to N(0,\theta^2)$. To find a confidence interval for θ, $\frac{\sqrt{n}(\widehat{\theta}-\theta)}{\theta} \to N(0,1)$.

$$1-\alpha = P\left(-z_{\alpha/2} < \frac{\sqrt{n}(\widehat{\theta}-\theta)}{\theta} < z_{\alpha/2}\right) = P\left(\frac{\widehat{\theta}}{1+\frac{z_{\alpha/2}}{\sqrt{n}}} < \theta < \frac{\widehat{\theta}}{1-\frac{z_{\alpha/2}}{\sqrt{n}}}\right)$$

What if $I(\theta)$ is more complicated? $\sqrt{n}(\widehat{\theta}-\theta)\sqrt{I(\theta)} \to N(0,1)$, and $\sqrt{n}(\widehat{\theta}-\theta)\sqrt{I(\widehat{\theta})} \to N(0,1)$, because $\sqrt{n}(\widehat{\theta}-\theta)\sqrt{I(\widehat{\theta})} = \sqrt{n}(\widehat{\theta}-\theta)\sqrt{I(\theta)}\sqrt{\frac{I(\widehat{\theta})}{I(\theta)}}$. Since $\widehat{\theta} \xrightarrow{P} \theta$, then $I(\widehat{\theta}) \xrightarrow{P} I(\theta)$. $I(\theta) = -E\left[\frac{d^2\log f(x|\theta)}{d\theta^2}\right]$. If the above expression is hard to find, then get a consistent estimator of it.

$$-\frac{1}{n}\left[\frac{d^2\log L}{d\theta^2}\right] = -\frac{1}{n}\sum_{i=1}^n\frac{d^2\log f(x_i|\theta)}{d\theta^2} \xrightarrow{P} I(\theta).$$

What about

$$-\frac{1}{n}\left[\frac{d^2\log L}{d\theta^2}\right]_{\theta=\widehat{\theta}} \xrightarrow{P} I(\theta)?$$

Theorem: If $x_n \xrightarrow{D} x$, and $\widehat{\theta} \xrightarrow{P} \theta$, then $h(x_n,\widehat{\theta}) \xrightarrow{D} h(x,\theta)$. If $x_n \xrightarrow{P} a$ and $\widehat{\theta} \xrightarrow{P} \theta$, then $h(x,\widehat{\theta}) \xrightarrow{P} h(a,\theta)$.

Important Result:

$$\sqrt{n}(\widehat{\theta}-\theta)\left[-\frac{1}{n}\frac{d^2\log L}{d\theta^2}\right]_{\theta=\widehat{\theta}} \to N(0,1).$$

You do not have to find the expected value. Let $y_1, y_2, ..., y_n$ be iid random variables. $E(y_i) = \mu$ and $E(\bar{y}) = \mu$. Then, $\bar{y}$ is a consistent estimator of μ. For large n,

$$\widehat{\theta} \sim N\left(\theta, \left[\frac{1}{-n\frac{d^2 \log L}{d\theta^2}}\right]_{\theta=\widehat{\theta}}\right).$$

14.21 Midterm Exam and Answers

The median score was 51, and the range of the scores was 30-64. Both the midterm exam and the final exam will count as 75% of your grade.

Instructions: You may use a calculator and bring one small note card with your notes on it. Answer any six problems out of seven.

1. Consider a random sample of size n from $U(0, \theta)$ distribution. Derive the mle of θ. Derive an unbiased estimator for θ.

   Solution: $f(x, \theta) = \frac{1}{\theta}, 0 < x < \theta$.

   $$L(\theta|\underline{x}) = \prod_{i=1}^{n} f(x_i|\theta) = \frac{1}{\theta^n}, 0 < x_i < \theta.$$

   θ is maximized when $\widehat{\theta} = \max(x_1, x_2, ..., x_n) = x_{(n)}$. We can not use $\bar{x}$ because it may fall to the left of $x_{(n)}$.

   $$L(\theta|\underline{x}) = \begin{cases} \frac{1}{\theta^n}, & \text{if } \theta > x_{(n)}. \\ 0, & \text{otherwise.} \end{cases}$$

   Thus, the mle is $\widehat{\theta} = x_{(n)}$. For the second part, let $y = x_{(n)}$. Then,

   $$g(y) = nF(y)^{n-1}f(y) = \frac{ny^{n-1}}{\theta^{n-1}}\frac{1}{\theta} = \frac{ny^{n-1}}{\theta^n}.$$

   $$E(x_{(n)}) = E(y) = \int_0^\theta \frac{yny^{n-1}}{\theta^n}\, dy = \frac{n}{\theta^n}\int_0^\theta y^n\, dy = \frac{n}{n+1}\theta = E(\widehat{\theta}) \Rightarrow \widehat{\theta}^* = \frac{n+1}{n}\widehat{\theta} \Rightarrow E(\widehat{\theta}^*) = \theta.$$

2. Consider a random sample of size n from $N(\mu_1, \sigma^2)$ distribution and a random sample of size m from $N(\mu_2, 2\sigma^2)$ distribution where σ is unknown. Derive a $(1-\alpha)100\%$ confidence interval of $\mu_1 - \mu_2$. Solution: We know that $\frac{(n-1)s_1^2}{\sigma^2} \sim \chi^2(n-1)$ and $\frac{(m-1)s_2^2}{2\sigma^2} \sim \chi^2(m-1)$, and

   $$\frac{(n-1)s_1^2}{\sigma^2} + \frac{(m-1)s_2^2}{2\sigma^2} \sim \chi^2(n+m-2).$$

$$s_p^2 = \frac{(n-1)s_1^2 + \frac{(m-1)s_2^2}{2}}{n+m-2}$$

is unbiased for σ^2. s_1^2 is unbiased for σ^2 and $\frac{s_2^2}{2}$ is unbiased for σ^2.

$$\bar{x} - \bar{y} \sim N\left(\mu_1 - \mu_2, \frac{\sigma^2}{n} + \frac{2\sigma^2}{m}\right),$$

$$\frac{\frac{\bar{x} - \bar{y} - (\mu_1 - \mu_2)}{\sqrt{\frac{\sigma^2}{n} + \frac{2\sigma^2}{m}}}}{\sqrt{\frac{s_p^2}{\sigma^2}}} \sim t.$$

3. Let $(y_1, y_2, ..., y_k)$ be multinomial$(n, p_1, p_2, ..., p_k)$. Also, let $Q_{k-1} = \sum(y_i - np_i)^2/(np_i)$. Prove that for $k = 2$, the asymptotic distribution of Q_{k-1} is $\chi^2(1)$. Solution:

$$Q_1 = \frac{(y_1 - np_1)^2}{np_1} + \frac{(y_2 - np_2)^2}{np_2}.$$

We know that $y_1 + y_2 = n$ and $p_1 + p_2 = 1$. Then,

$$\frac{(y_1 - np_1)^2}{np_1} + \frac{(n - y_1 - n(1-p_1))^2}{n(1-p_1)} = \frac{y_1^2 - 2np_1y_1 + n^2p_1^2}{np_1} + \frac{(n - y_1 - n + np_1)^2}{n(1-p_1)} =$$

$$\frac{(y_1^2 - 2np_1y_1 + n^2p_1^2)(1-p_1)}{np_1(1-p_1)} + \frac{(y_1^2 - 2ny_1p_1 + n^2p_1^2)p_1}{n(1-p_1)p_1} =$$

$$\frac{y_1^2 - 2np_1y_1 + n^2p_1^2 - y_1^2p_1 + 2np_1^2y_1 - n^2p_1^3 + y_1^2p_1 - 2ny_1p_1^2 + n^2p_1^3}{n(1-p_1)p_1} =$$

$$\frac{y_1^2 - 2np_1y_1 + n^2p_1^2}{n(1-p_1)p_1} = \frac{(y_1 - np_1)^2}{n(1-p_1)p_1} \sim \chi^2(1)$$

because it is the square of a standard normal distribution.

4. Let $x_1, x_2, ..., x_{10}$ be a random sample of size 10 from the $Poisson(\theta)$ distribution. Give a test of exact size 0.125 for $H_0 : \theta = 0.5$ against $H_1 : \theta < 0.5$. Find the power of this test for $H_1 : \theta = 0.25$. Solution: Reject H_0 if $\bar{x} < c \Rightarrow y \leq c^*$. $y = \sum_{i=1}^{10} x_i$, $y|H_0 \sim Poisson(5)$. Find c^* such that $P(y \leq c^*|H_0) = 0.125$.

c^*	$P(y \leq c^*)$
0	e^{-5}
1	$e^{-5}(1+5)$
2	$e^{-5}\left(1 + 5 + \frac{5^2}{2!}\right) = 0.125$

$y|H_1 \sim Poisson(2.5)$. The power is given by the expression

$$P(\text{Reject } H_0|H_1 \text{ true}) = P(y \leq 2|H_1) = e^{-2.5}\left(1 + 2.5 + \frac{(2.5)^2}{2!}\right) = 0.544.$$

5. Consider a random sample of size n from the normal distribution with a mean of θ and a variance of θ. Derive the minimal set of sufficient statistics. Is it a complete set? Derive the mle of θ. Is $\bar{x}$ the unbiased minimum variance estimator? Give your reasons. Solution:

$$f(x,\theta) = \frac{1}{\sqrt{2\pi\theta}} e^{-\frac{(x-\theta)^2}{2\theta}}$$

$$\frac{1}{\sqrt{2\pi\theta}} e^{-\frac{x^2}{2\theta}-\frac{\theta}{2}+x} e^{-\frac{1}{2}\log\theta}.$$

This is the regular exponential family with $T = \sum x_i^2$ which is the *minimum* complete statistic. The mle to the solution is quadratic.

$$\log L = -\sum_{i=1}^{n} \frac{(x_i-\bar{x})^2}{2\theta} - \frac{n(\bar{x}-\theta)^2}{2\theta} - n\log\sqrt{2\pi\theta} = -\sum_{i=1}^{n} \frac{(x_i-\bar{x})^2}{2\theta} - \frac{n(\bar{x}-\theta)^2}{2\theta} - \frac{n}{2}\log(2\pi\theta) =$$

$$-\sum_{i=1}^{n} \frac{(x_i-\bar{x})^2}{2\theta} - \frac{n(\bar{x}^2-2\bar{x}\theta+\theta^2)}{2\theta} - \frac{n}{2}\log 2\pi\theta, \quad \frac{d\log L}{d\theta} = \sum_{i=1}^{n} \frac{(x_i-\bar{x})^2}{2\theta^2} + \frac{n\bar{x}^2}{2\theta^2} - \frac{n}{2} - \frac{n}{2(2\pi\theta)} = 0.$$

$$\sum_{i=1}^{n}(x_i-\bar{x})^2 + n\bar{x}^2 - n\theta^2 - \frac{n\theta}{2\pi} = \overbrace{n\theta^2}^{a} + \overbrace{\frac{n\theta}{2\pi}}^{b} - \overbrace{\left[n\bar{x}^2 + \sum(x_i-\bar{x})^2\right]}^{c} = 0.$$

Next, solve for the roots using the quadratic equation

$$\frac{-b \pm \sqrt{b^2-4ac}}{2a}, \quad \frac{-\frac{n}{2\pi} \pm \sqrt{\frac{n^2}{4\pi^2} + 4n\left[n\bar{x}^2 + \sum(x_i-\bar{x})^2\right]}}{2n}.$$

But, since the variance must be positive, the mle is

$$\frac{-\frac{n}{2\pi} + \sqrt{\frac{n^2}{4\pi^2} + 4n\left[n\bar{x}^2 + \sum(x_i-\bar{x})^2\right]}}{2n}.$$

Can $\bar{x}$ be the unbiased minimum variance estimator? No, because it is not a function of T and it can be negative.

6. Let $\widehat{\theta}_i, i = 1,2,...,k$ be k independent unbiased estimators of θ with a known variance $Var(\widehat{\theta}_i) = \sigma_i^2, i = 1,2,...,k$. Derive the best linear unbiased estimator of θ in the class of $\sum a_i\widehat{\theta}_i + b$. Solution:

$$\widehat{\theta} = \frac{\sum \frac{\widehat{\theta}_i}{\sigma_i^2}}{\sum_{j=1}^{k}\frac{1}{\sigma_j^2}}, \quad \sum a_i\widehat{\theta}_i + b, \quad \theta = E\left[\sum a_i\widehat{\theta}_i + b\right], \forall\theta \Rightarrow b = 0, \text{ and } \sum a_i = 1.$$

$a_i = \frac{\frac{1}{\sigma_i^2}}{\sum\frac{1}{\sigma_j^2}}$ We need to minimize the variance $Var\left(\sum a_i\widehat{\theta}_i\right) = \sum a_i^2\sigma_i^2$ such that $\sum a_i = 1$.

7. If x_1 and x_2 are the random sample from $exp(\theta)$, find the joint pdf of $y_1 = x_1 + x_2$ and $y_2 = x_2$. Since y_2 is an unbiased estimator of θ, use it to find the unbiased minimum variance estimator of θ and compare its variance to the variance of y_2. Partial Solution:

$$f(x,\theta) = \frac{1}{\theta}e^{-\frac{x}{\theta}}, 0 < x < \infty, \;\; g(x_1, x_2) = \frac{1}{\theta^2}e^{-\frac{x_1}{\theta}}e^{-\frac{x_2}{\theta}} = \frac{1}{\theta^2}e^{-\frac{x_1+x_2}{\theta}}.$$

$x_1 = y_1 - y_2$ and $x_2 = y_2$. The Jacobian $|J| = 1$.

$$h(y_1, y_2) = \frac{1}{\theta^2}e^{-\frac{y_1-y_2+y_2}{\theta}}, 0 < y_2 < y_1 < \infty, \;\; h(y_1, y_2) = \frac{1}{\theta^2}e^{-\frac{y_1}{\theta}}.$$

$$h_2(y_2) = \int_{-\infty}^{\infty} h(y_1, y_2)\, dy_1 = \int_{y_2}^{\infty} \frac{1}{\theta^2}e^{-\frac{y_1}{\theta}}\, dy_1 = -\frac{1}{\theta}e^{-\frac{y_1}{\theta}}\Big|_{y_2}^{\infty} = \frac{1}{\theta}e^{-\frac{y_1}{\theta}}.$$

$$E(y_2) = \int_{-\infty}^{\infty} y_2 h_2(y_2)\, dy_2 = \int_0^{\infty} \frac{y_2 e^{-\frac{y_2}{\theta}}}{\theta}\, dy_2.$$

Integrate by parts. Let $u = y_2, du = dy_2$ and $dv = \frac{e^{-\frac{y_2}{\theta}}}{\theta}, v = -e^{-\frac{y_2}{\theta}}$.

$$-y_2 e^{-\frac{y_2}{\theta}}\Big|_0^{\infty} + \int_0^{\infty} e^{-\frac{y_2}{\theta}}\, dy_2 = \theta \Rightarrow \text{ unbiased.}$$

Here are some important points:

- x has the pdf $f(x|\theta)$. $T = T(x_1, x_2, ..., x_n)$ is sufficient for θ. Is T complete? $g(t|\theta)$, the pdf of T must be a complete family. But, for the regular exponential family of $f(x|\theta)$ will work. Suppose we have $T = x_{(n)}$. Then,

$$g(t|\theta) = \frac{nt^{n-1}}{\theta^n}, 0 < t < \theta, \;\; E[u(T)] = 0, \;\; n\int_0^{\theta} \frac{u(t)t^{n-1}}{\theta^n}dt = 0.$$

- Given $\widehat{\theta} = u(x_1, x_2, ..., x_n)$. Any estimator $\widehat{\theta}$ must be a completely specified function of the sample. $\sum \frac{(x_i-\mu)^2}{n}$ is not an estimator because μ is unknown.
- Given $f(x|\theta)$ is the pdf of x for a given parameter θ. $E(x) = \theta$ and $E(x|\theta) = \theta$ are true. But, $E(x|\widehat{\theta}) = \widehat{\theta}$ is not true. You need to find the conditional distribution of x given $\widehat{\theta}$.
- Given $z \sim N(0, 1)$ and $y \sim \chi^2(r)$. y and z are independent. Then, the student's t-distribution is

$$T = \frac{z}{\left(\frac{y}{r}\right)^{1/2}} \sim t(r).$$

14.22 Robust Estimation

An estimator is *robust* if it has good properties for a wide variety of distributions. Assume that $x \sim N(\mu, \sigma^2)$. The mle of μ is $\widehat{\mu} = \bar{x}$. For the mle,

1. If $x \sim N(\theta, \sigma^2)$, then we minimize $\sum (x_i - \theta)^2$.
2. If $x \sim$ doubly $exp(\theta)$, then $f(x|\theta) = e^{-|x-\theta|}, -\infty < x < \infty$. We minimize $\sum |x_i - \theta|$.

Consider the likelihood function $L(\theta|x) = \prod_{i=1}^n f(x_i|\theta) = \prod_{i=1}^n f(x_i - \theta)$ with the location parameter θ. $\log L = \sum \log f(x_i|\theta) = -\sum_{i=1}^n p(x_i - \theta) = \sum_{i=1}^n \log f(x_i - \theta)$, where $p(x) = -\log f(x)$. The mle is $\frac{d \log L}{d\theta} = \sum \psi(x_i - \theta)$, $\psi(x_i - \theta) = -\frac{dp(x_i - \theta)}{d\theta}$.

Example:

	$p(x)$	$\psi(x)$
Normal	$c + \frac{x^2}{2\sigma^2}$	$\frac{x}{\sigma^2}$
Double Exp	$c + \log \lvert x \rvert$	$\begin{cases} -1, & \text{if } x < 0. \\ 1, & \text{if } x > 0. \end{cases}$
Cauchy	$c + \log(1 + x^2)$	$\frac{2x}{1+x^2}$

The *Huber* ψ function is given by

$$\psi(x) = \begin{cases} -k, & \text{if } x < -k. \\ x, & \text{if } -k < x < k. \\ k, & \text{if } x > k. \end{cases}$$

We minimize $\sum \psi(x_i - \theta)$ for the estimate of the location parameter θ. For the normal case, say $\psi(x) = x$, σ^2 does not matter. It is truncating at

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------|----------------------------------|-------
     -k                                  k
```

It takes care of outliers, also. Start with some θ_0 to minimize $\sum \psi(x_i - \theta_0) = 0$. Then solve

$$\widehat{\theta} = \sum_{i=1}^{n-r_1-r_2} \frac{x_i + k(r_2 - r_1)}{n - r_1 - r_2},$$

$x_1 - \theta_0, x_2 - \theta_0, ..., x_n - \theta_0$.

$$\sum_{i=1}^{n} (x_i - \theta_0) = 0 \Rightarrow \sum_{i=r_1+1}^{n-r_2+1} (x_i - \theta_0) - kr_1 + kr_2 = 0 \Rightarrow \theta_0 = \frac{\sum_{i=1}^{n-r_1-r_2} x_i + k(r_2 - r_1)}{n - r_1 - r_2}$$

is called a *trimmed mean* of the middle values. We need to take care of the scale parameter by solving $\sum \psi\left(\frac{x_i - \theta}{d}\right) = 0$ where d is some robust estimator of the scale parameter. $d = median|x_i - med(x_j)|/0.6745$, and the expected value is $E(d|\text{Normal}) = \sigma$. What should be k? $k = 1.5$ or $k = 2$ in the Huber function.

14.23 Best Critical Regions

Let $\underline{x} = (x_1, x_2, ..., x_n)^T$. Then, C is the *best critical region* of size α for $H_0 : \theta = \theta_0$ against $H_1 : \theta = \theta_1$ if $P(\underline{x} \in C|H_0) = \alpha$ for any other critical region of size A of size α. $P(\underline{x} \in C|H_1) \geq P(\underline{x} \in A|H_1)$ (the power).

Neyman-Pearson Lemma Let $x_1, x_2, ..., x_n$ be a random sample from a distribution with the pdf $f(x|\theta), \theta \in \Omega$. Let $L(\theta|\underline{x}) = \prod_{i=1}^{n} f(x_i|\theta)$ be the likelihood function. If θ_0 and θ_1 are two distinct values of θ and let k be a positive number such that

1. $\frac{L(\theta_0|\underline{x})}{L(\theta_1|\underline{x})} \leq k$ for $\underline{x} \in C$.
2. $\frac{L(\theta_0|\underline{x})}{L(\theta_1|\underline{x})} \geq k$ for $\underline{x} \in C'$.
3. $\alpha = P(\underline{x} \in C|H_0)$.

Then, C is the best critical region (BCR) of size α for $H_0 : \theta = \theta_0$, versus $H_1 : \theta = \theta_1$. **Proof:** $\alpha = P(x \in C|H_0) = \int_{\underline{x} \in C} L(\theta_0|\underline{x})\, d\underline{x}$. Also, $\alpha = \int_{\underline{x} \in A} L(\theta_0|\underline{x})\, d\underline{x}$. Then,

$$\int_{CA'} L(\theta_0|\underline{x})\, d\underline{x} + \int_{AC'} L(\theta_0|\underline{x})\, d\underline{x}.$$

$$k_C(\theta_1) = P(x \in C|H_1) = \int_C L(\theta_1|\underline{x})\, d\underline{x} = \int_{CA'} L(\theta_1|\underline{x}) d\underline{x} + \int_{CA} L(\theta_1|\underline{x}) d\underline{x}.$$

Then, prove that $k_C(\theta_1) \geq k_A(\theta_1)$.

$$\int_{CA'} L(\theta_1|\underline{x})\, d\underline{x} \geq \int_{CA'} \frac{L(\theta_0|\underline{x})}{k}\, d\underline{x} = \int_{AC'} \frac{L(\theta_0|\underline{x})}{k}\, d\underline{x} \geq \int_{AC'} L(\theta_1|\underline{x})\, d\underline{x}.$$

Then,

$$k_C(\theta_1) \geq \int_{AC'} L(\theta_1|\underline{x})\, d\underline{x} + \int_{AC} L(\theta_1|\underline{x})\, d\underline{x} = \int_A L(\theta_1|\underline{x})\, d\underline{x} = k_A(\theta_1).$$

So, $k_C(\theta_1) \geq k_A(\theta_1)$ for any A of size α.

Example: $x \sim N(\theta, \sigma^2)$, where σ is known. The hypotheses are $H_0 : \theta = \theta_0$ versus $H_1 : \theta = \theta_1$.

$$L(\theta|\underline{x}) = \left(\frac{1}{\sqrt{2\pi}\sigma}\right)^n e^{-\frac{\sum(x_i-\theta)^2}{2\sigma^2}}.$$

Find the BCR of size α.

$$\frac{L(\theta_0|\underline{x})}{L(\theta_1|\underline{x})} \leq k \Rightarrow \frac{e^{-\frac{\sum(x_i-\theta_0)^2}{2\sigma^2}}}{e^{-\frac{\sum(x_i-\theta_1)^2}{2\sigma^2}}} \leq k.$$

Consider the property,

$$\sum_{i=1}^{n}(x_i-\theta)^2=\sum_{i=1}^{n}(x_i-\bar{x})^2+n(\bar{x}-\theta)^2 \Rightarrow e^{-\frac{n(\bar{x}-\theta_0)^2}{2\sigma^2}+\frac{n(\bar{x}-\theta_1)^2}{2\sigma^2}} \leq k \Rightarrow e^{\frac{\bar{x}(\theta_0-\theta_1)}{\sigma^2}} \leq k^*,$$

$\frac{\bar{x}(\theta_0-\theta_1)}{\sigma^2} < \log k^*$. If $\theta_1 > \theta_0$, then $\bar{x} \geq c$. If $\theta_1 < \theta_0$ then $\bar{x} \leq c$. How do we find c? Fix α and find c from

$$\alpha = P(\text{Reject } H_0|H_0) = P(\bar{x} > c|\theta_0) = P\left(\frac{\bar{x}-\theta_0}{\sigma_{\bar{x}}} > \frac{c-\theta_0}{\sigma_{\bar{x}}}\middle|\theta_0\right) = P\left(z > \frac{(c-\theta_0)\sqrt{n}}{\sigma}\right).$$

From the tables, $\alpha = P(Z > z_\alpha)$. Note here that $\sigma_{\bar{x}} = \frac{\sigma}{n}$. See Figure 14.13. So, the BCR is given by $\bar{x} > c$ where

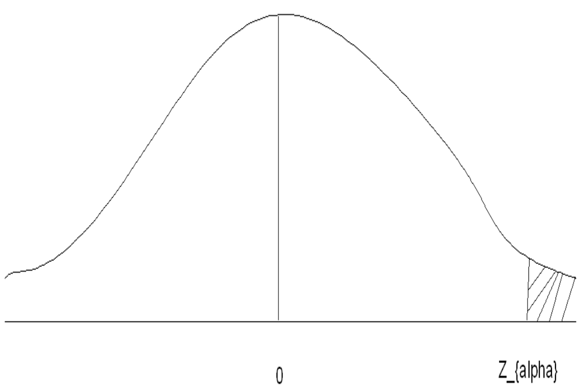


Figure 14.13: The cut-off value c determination and the Type I error.

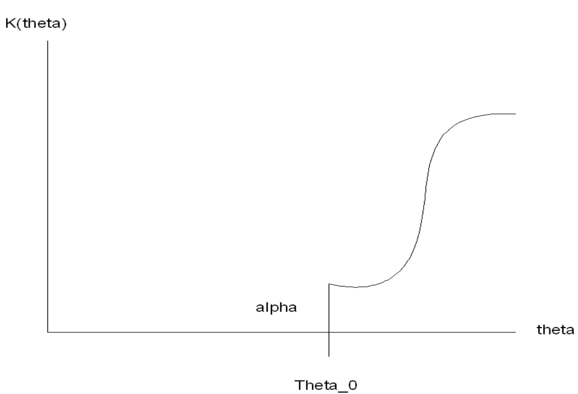


Figure 14.14: The curve of the power calculation.

$\frac{(c-\theta_0)\sqrt{n}}{\sigma} = z_\alpha \Rightarrow c = \frac{\sigma}{\sqrt{n}}z_\alpha + \theta_0$. The statistical power is $k(\theta_1) = P(\text{Reject } H_0|H_1) = P(\bar{x} > c|\theta_1)$. See Figure 14.14.

14.24 Uniformly Most Powerful Test

This section covers the UMPT for composite H_1. Suppose we have $H_0 : \theta = \theta_0$ versus $H_1 : \theta \in \Omega$. If the BCR for $H_0 : \theta = \theta_0$ against $H_1 : \theta = \theta_1 \in \Omega_1$ does not depend on θ_1, then the test is uniformly most powerful

(UMP) for $H_1 : \theta \in \Omega_1$.

Example: Suppose that $x \sim N(\theta, \sigma^2)$. We wish to test $H_0 : \theta = \theta_0$, versus $H_1 : \theta > \theta_0$. The BCR for $H_0 : \theta = \theta_0$ and $H_1 : \theta = \theta_1 > \theta_0$ is reject H_0 if $\bar{x} > c = \theta_0 + \frac{z_\alpha \sigma}{\sqrt{n}}$ which is the same test for any $\theta > \theta_0$.

Example: Suppose that $x \sim N(\theta, \sigma^2)$. We wish to test $H_0 : \theta = \theta_0$, versus $H_1 : \theta < \theta_0$. What is the BCR for $\theta_1 < \theta_0$? Reject H_0 if $\bar{x} < c = \theta_0 - \frac{z_\alpha \sigma}{\sqrt{n}}$.

Example: Suppose that $x \sim N(0, \sigma^2)$. We wish to test $H_0 : \theta = \theta_0$, versus $H_1 : \theta \neq \theta_0$. What is the BCR for $\theta_1 \neq \theta_0$? This has two different critical regions. The BCR depends on the alternative hypothesis. When this happens, use the likelihood ratio test. To calculate p-values for the test H_0 if $\bar{x} > c$ where $x \sim N\left(\theta, \frac{\sigma^2}{n}\right)$ take a sample and compute $\bar{x}$. Then, $p = P(\bar{X} \geq \bar{x})$. We reject H_0 for any $\alpha \geq p$.

Example: Take $p = 0.004$. Reject H_0 for any $\alpha \geq 0.004$.

Example: Consider $H_1 : \theta \neq \theta_0$. If $\bar{x}$ is the value of $\bar{X}$ for a given sample and if $\bar{x} > \theta_0$, then $p = 2P(\bar{X} > \bar{x}|H_0)$. Consider an unbiased test for $H_0 : \theta = \theta_0$ versus $H_1 : \theta \in \Omega_1$. The power is $k(\theta) = P(\text{Reject } H_0|H_1)$. The test is unbiased if $k(\theta) \geq k(\theta_0) \forall \theta \in \Omega_1$ where $k(\theta_0) = \alpha = P(\text{Reject } H_0|H_0)$.

Example: Suppose we have the normal distribution where $x \sim N(\theta, \sigma^2)$ where σ is known. We wish to test for $H_0 : \theta = \theta_0$ versus $H_1 : \theta \neq \theta_0$. We have the BCR for $H_1 : \theta > \theta_0$ as being $\bar{x} > c = \theta_0 + \frac{z_\alpha \sigma}{\sqrt{n}}$. We also have the BCR for $H_1 : \theta < \theta_0$ as being $\bar{x} < c = \theta_0 - \frac{z_\alpha \sigma}{\sqrt{n}}$. For the first critical region,

$$k(\theta) = P\left(\text{Reject } H_0|H_1\right) = P\left(\bar{x} > \theta_0 + \frac{z_\alpha \sigma}{\sqrt{n}}\right) = P\left(\frac{\bar{x} - \theta}{\sigma_{\bar{x}}} > \frac{\theta_0 - \theta}{\sigma_{\bar{x}}} + z_\alpha \middle| \theta > \theta_0\right) =$$

$$P\left(z > z_\alpha + \frac{\theta_0 - \theta}{\sigma_{\bar{x}}}\right) = 1 - \Phi\left(z_\alpha + \frac{\theta_0 - \theta}{\sigma_{\bar{x}}}\right).$$

Suppose we wish to test $H_0 : \theta = \theta_0$ versus $H_1 : \theta \neq \theta_0$. Reject H_0 if $z = \frac{\bar{x} - \theta_0}{\sigma_{\bar{x}}} < -z_{\alpha/2}$ or if $z = \frac{\bar{x} - \theta_0}{\sigma_{\bar{x}}} > z_{\alpha/2}$. Then, reject H_0 if $\bar{x} > \theta_0 + z_{\alpha/2} \frac{\sigma}{\sqrt{n}}$ or $\bar{x} < \theta_0 - z_{\alpha/2} \frac{\sigma}{\sqrt{n}}$. Now,

$$k(\theta) = P(\text{Reject } H_0|H_1) = P\left(\bar{x} > \theta_0 + z_{\alpha/2} \frac{\sigma}{\sqrt{n}} \middle| \theta\right) + P\left(\bar{x} < \theta_0 - z_{\alpha/2} \frac{\sigma}{\sqrt{n}} \middle| \theta\right) =$$

$$P\left(z > z_{\alpha/2} + \frac{(\theta_0 - \theta)\sqrt{n}}{\sigma}\right) + P\left(z < -z_{\alpha/2} + \frac{(\theta_0 - \theta)\sqrt{n}}{\sigma}\right) \geq \alpha \Rightarrow \text{ unbiased.}$$

We cannot choose z_{α_1} and z_{α_2}. It may be biased.

14.25 Likelihood Ratio Test

The Neyman lemma only gives a test for simple H_0. If there is more than one parameter, then the test does not work.

Example: Suppose we have the normal distribution $N(\theta_1, \theta_2)$. We wish to test $H_0 : \theta_1 = 0$ versus $H_1 : \theta_1 > 0$. Under the Neyman-Person lemma, $\bar{x} > c$ depends on θ_2. $\bar{x}|H_0 \sim N\left(0, \frac{\theta_2}{n}\right)$. Thus, we need to use the likelihood ratio test. Suppose that x had the pdf $f(x|\theta), \theta \in \Omega$. $\theta' = (\theta_1, \theta_2, ..., \theta_k)$. We wish to test $H_0 : \theta \in W \subset \Omega$ versus $H_1 : \theta \in \Omega$. To find the mle of θ, under Ω we have the mle $\widehat{\theta}_\Omega$, and under W we have the mle $\widehat{\theta}_W$, $L(\theta|\underline{x}) = \prod_{i=1}^n f(x_i|\theta)$. $0 \leq \lambda = \frac{L(\widehat{\theta}_W|\underline{x})}{L(\widehat{\theta}_\Omega|\underline{x})} \leq 1$. Reject H_0 for small values of λ where $\lambda \leq \lambda_0$.

How do we find λ_0? Fix α to find λ_0. $\alpha = P(\lambda \leq \lambda_0 | H_0)$. This must simplify to a known test statistic. If you can not simply it, then it's know that for large n, $-2\log\lambda \to \chi^2(k-r)$ where r is the dimension of W and $k-r$ is the number of parameters specified under H_0 which is also the reduction in dimension of Ω. Very useful.

Example: Let $x \sim N(\theta_1, \theta_2)$. Test test the hypotheses $H_0 : \theta_1 = 0$ versus $H_1 : \theta_1 \neq 0$. The likelihood function is

$$L(\theta|\underline{x}) = \frac{1}{(2\pi\theta_2)^{n/2}} e^{-\frac{\sum(x_i-\theta_1)^2}{2\theta_2}}, \ \ \Omega : \widehat{\theta}_1 = \bar{x}, \ \ \widehat{\theta}_2 = s^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2,$$

$$L(\widehat{\theta}_\Omega|\underline{x}) = \frac{1}{(2\pi s^2)^{n/2}} e^{-\frac{\sum_{i=1}^n (x_i-\bar{x})^2}{2s^2}} = \frac{e^{-\frac{n}{2}}}{(2\pi)^{n/2}s^n} = L(\widehat{\theta}_\Omega|\underline{x}).$$

Under $W : \theta_1 = 0; \widehat{\theta}_{2W} = \frac{\sum_{i=1}^n x_i^2}{n}$.

$$L(\theta|\underline{x}) = \left(\frac{1}{2\pi\theta_2}\right)^{n/2} e^{-\frac{\sum x_i^2}{2\theta_2}} \Rightarrow L(\widehat{\theta}_W|\underline{x}) = \frac{e^{-\frac{n}{2}}}{(2\pi)^{n/2}}\frac{1}{\widehat{\theta}_{2W}}.$$

$$\lambda = \frac{L(\widehat{\theta}_W|\underline{x})}{L(\widehat{\theta}_\Omega|\underline{x})} = \left(\frac{s^2}{\frac{\sum_{i=1}^n x_i^2}{n}}\right)^{n/2} = \left(\frac{\sum_{i=1}^n (x_i-\bar{x})^2}{\sum_{i=1}^n x_i^2}\right) = \left(\frac{\sum_{i=1}^n (x_i-\bar{x})^2}{\sum_{i=1}^n (x_i-\bar{x}+\bar{x})^2}\right) = \left(\frac{\sum_{i=1}^n (x_i-\bar{x})^2}{\sum_{i=1}^n (x_i-\bar{x})^2 + n\bar{x}^2}\right).$$

Under $H_0 : \frac{\sqrt{n}}{s}\bar{x} \sim t(n-1)$.

$$\frac{1}{\left[1 + \frac{n\bar{x}^2}{\sum_{i=1}^n (x_i-\bar{x})^2}\right]^{n/2}} \leq \lambda_0.$$

Then, $\frac{n\bar{x}^2}{\sum(x_i-\bar{x})^2} \geq c \Rightarrow \frac{\sqrt{n}\bar{x}}{s} < -c^*$ or $> c^*$. $t = \frac{n\bar{x}}{s}$. Reject H_0 if $t < -t_{\alpha/2}(r)$ or if $t > t_{\alpha/2}(r)$ where $r = n-1$.

Example: Suppose that $x \sim N(\theta_1, \theta_2)$. We wish to test $H_0 : \theta_2 = \theta_2^0$ where θ_2^0 is a specified value. The likelihood function is

$$L(\theta|\underline{x}) = \frac{1}{(2\pi\theta_2)^{n/2}} e^{-\frac{\sum_{i=1}^n (x_i-\theta_1)^2}{2\theta_2}}, \ \ \Omega : \widehat{\theta}_1 = \bar{x}; \widehat{\theta}_2 = s^2, \ \ L(\widehat{\theta}_\Omega|\underline{x}) = \frac{e^{-n/2}}{(2\pi)^{n/2}}\frac{1}{s^n}$$

$$W : \widehat{\theta}_1 = \bar{x}, \ \ L(\widehat{\theta}_W|\underline{x}) = \frac{1}{(2\pi\theta_2^0)^{n/2}} e^{-\frac{\sum_{i=1}^n (x_i-\bar{x})^2}{2\theta_2^0}},$$

$$\lambda = \left(\frac{s^2}{\theta_2^0}\right)^{n/2} e^{-\frac{ns^2}{2\theta_2^0}} e^{n/2} \leq \lambda_0 \Rightarrow \overbrace{\left(\frac{ns^2}{\theta_2^0}\right)^{n/2}}^{\chi^2(n-1)} e^{-\frac{ns^2}{2\theta_2^0}} \leq \lambda_0^*, \ \ y = \frac{ns^2}{\theta_2^0}, \ \ h(y) = e^{-\frac{y}{2}}y^n \Rightarrow y \leq c_1 \text{ or } y \geq c_2.$$

We need to find c_1 and c_2 such that $\alpha = P(y \leq c_1) + P(y \geq c_2)$ and such that $e^{-\frac{c_1}{2}}c_1^{n/2} = e^{-\frac{c_2}{2}}c_2^{n/2}$. See Figure 14.15. This does not imply that the lengths are equal. The shortest confidence interval for θ_2 is

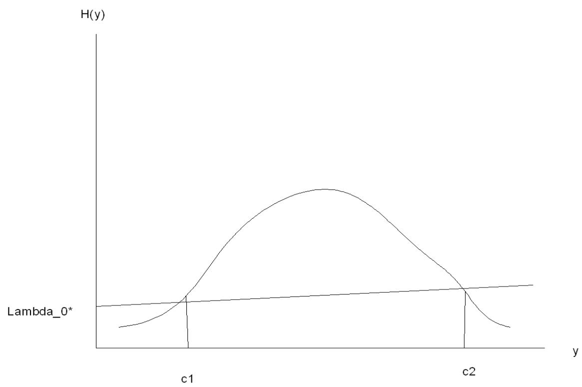


Figure 14.15: The curve for determining the value of λ_0^*.

$e^{-\frac{c_1}{2}} c_1^{\frac{n+1}{2}} = e^{-\frac{c_2}{2}} c_2^{\frac{n+1}{2}}$.

Example: Let $x \sim N(\theta_1, 1)$. We wish to test $H_0 : \theta_1 = 0$ versus $H_1 : \theta_1 > 0$ or $H_1 : \theta_1 < 0$ or $H_1 : \theta_1 \neq 0$. Finding the power of the test involves the standard normal distribution. $\frac{\bar{x}}{\frac{1}{\sqrt{n}}} = \sqrt{n}\bar{x} \sim N(0,1)$ under H_0. If H_1 is true then, $x \sim N(\sqrt{n}\theta_1, 1)$. Subtract the two. The power for the t test where $x \sim N(\theta_1, \theta_2)$ is $H_0 : \theta_1 = 0$. $s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$, $t = \frac{\sqrt{n}\bar{x}}{s}$. If H_0 is true, then $\frac{(n-1)s^2}{\theta_2} \sim \chi^2(n-1)$ is always true. $\sqrt{n}\bar{x} \sim N(\theta_1, \theta_2)$. In the following case, the power does depend on both θ_1 and θ_2.

$$t = \frac{\frac{\sqrt{n}\bar{x}}{\sqrt{\theta_2}}}{\left(\frac{s^2}{\theta_2}\right)^{1/2}} = \frac{N\left(\frac{\sqrt{n}\theta_1}{\sqrt{\theta_2}}, 1\right)}{\sqrt{\frac{\chi^2(r)}{r}}}$$

is called a *non-central* t-distribution where the non-centrality parameter $\delta = \frac{\sqrt{n}\theta_1}{\sqrt{\theta_2}}$.

Definition: If $x \sim N(\delta, 1)$ and $y \sim x^2(r)$, and x and y are independent, then $t = \frac{x}{\sqrt{\frac{y}{r}}} \sim$ non-central $t(r)$ has a non-central t-distribution with r degrees of freedom and the non-centrality parameter δ.

14.26 Sequential Probability Ratio Test

The idea behind the sequential probability ratio test (SPRT) is to test sequentially, and at each step either of the following.

1. Reject H_0.
2. Reject H_1.
3. Continue sampling.

The hypotheses are $H_0 : \theta = \theta'$ versus $H_1 : \theta = \theta''$. The likelihood function $L(\theta|\underline{x}) = \prod_{i=1}^{n} f(x_i|\theta) = L(\theta, n), n = 1, 2, ...$ N is the stage at which the decision is reached and N is a random variable. We need to compare $E(N)$ with the fixed sample size for the same power.

$\lambda_n = \frac{L(\theta', n)}{L(\theta'', n)}$. Reject H_0 at the n-th stage if $\lambda_n \leq k_0$. Reject H_1 at the n-th stage if $\lambda_n \geq k_1$. Continue sampling if $k_0 < \lambda_n < k_1$. See Figure 14.16. We need to define the critical region. $c_n = \{\underline{x} : k_0 < \lambda_r < 1, r = 1, 2, ..., n-1; \lambda_n \leq k_0\}$. $B_n = \{\underline{x} : k_0 < \lambda_r < 1, r = 1, 2, ..., n-1; \lambda_1 \geq k_1\}$. The critical region C for

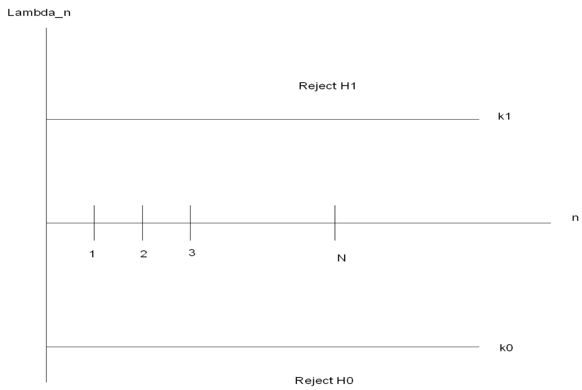


Figure 14.16: The critical regions for sequentially testing H_0 and H_1.

$H_0 : C = \bigcup_{n=1}^{\infty} C_n$. Similarly, $B = \bigcup_{n=1}^{\infty} B_n$. $\sum_{i=1}^{n} P(C_n) + \sum_{i=1}^{n} P(B_n) = 1$.

Questions:

1. What is the probability of continuing indefinitely? $P(N < \infty) = 1$.
2. What are the properties of N? (That is $E(N)$).

Example: Suppose $x \sim Bernoulli(\theta)$. We wish to test $H_0 : \theta = \frac{1}{2}$, versus $H_1 : \theta = \frac{3}{4}$. The likelihood function is

$$L(\theta|\underline{x}) = \theta^{\sum x_i}(1-\theta)^{n-\sum x_i}, \quad \lambda_n = \frac{\left(\frac{1}{2}\right)^{\sum x_i}\left(\frac{1}{2}\right)^{n-\sum x_i}}{\left(\frac{3}{4}\right)^{\sum x_i}\left(\frac{1}{4}\right)^{n-\sum x_i}}, \quad k_0 < \lambda_n < k_1 \Rightarrow c_0(n) < \sum x_i < c_1(n).$$

We fix α and β to find $c_0(n)$ and $c_1(n)$. See Figure 14.17.

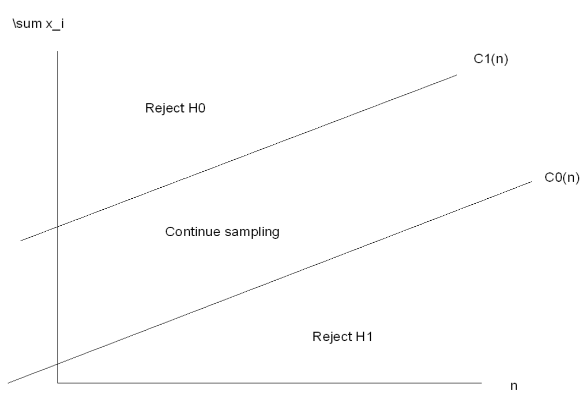


Figure 14.17: The critical regions for sequentially testing H_0 and H_1 in the Bernoulli example.

Given the likelihood ratio $\frac{L(\theta',n)}{L(\theta'',n)}$, how do we find k_0 and k_1? The relationship between (α, β) and (k_0, k_1) is such

1. $k_0 \geq \frac{\alpha}{1-\beta}$.
2. $k_1 \leq \frac{1-\alpha}{\beta}$.

Proof: $\alpha = P(\text{Reject } H_0|H_0) = \sum_n \int_{C_n} L(\theta', n)\, d\underline{x}$. Note that

$$d_n\, C_n, \frac{L(\theta', n)}{L(\theta'', n)} \le k_0 \Rightarrow \sum_n \int_{C_n} L(\theta', n)\, d\underline{x} \le k_0 \sum \int_{C_n} L(\theta'', n)\, d\underline{x} = k_0 P(\text{Reject } H_0|H_1) \Rightarrow \alpha \le k_0(1-\beta).$$

Now, to prove the second inequality above. $1 - \alpha = P(\text{Reject } H_1|H_0) = \sum \int_{B_n} L(\theta', n)\, d\underline{x}$. In B_n,

$$\frac{L(\theta', n)}{L(\theta'', n)} \ge k_1 \Rightarrow L(\theta', n) \ge k_1 L(\theta'', n).$$

$$\sum \int_{B_n} L(\theta', n)\, d\underline{x} \ge k_1 \sum \int_{B_n} L(\theta'', n)\, d\underline{x} = k_1 P(\text{Reject } H_1|H_1) \Rightarrow 1 - \alpha \ge k_1 \beta.$$

These results hold for any k_0 and k_1. Start with some α_a and β_a. We use $k_0 = \frac{\alpha_a}{1-\beta_a}$ and $k_1 = \frac{1-\alpha_a}{\beta_a}$. The actual α and β for k_0 and k_1 given above will be different from α_a and β_a. The result is $\alpha + \beta \le \alpha_a + \beta_a$. **proof:** $k_0 \ge \frac{\alpha}{1-\beta}$, $\frac{\alpha_a}{1-\beta_a} \ge \frac{\alpha}{1-\beta}$, $\alpha(1-\beta_a) \le \alpha_a(1-\beta)$, $k_1 \le \frac{1-\alpha}{\beta}$, $\frac{1-\alpha_a}{\beta_a} \le \frac{1-\alpha}{\beta} \Rightarrow \beta(1-\alpha_a) \le (1-\alpha)\beta_a$. Then adding, $\alpha + \beta \le \alpha_a + \beta_a$.

Example: Let $\alpha_a = 0.05$ and $\beta_a = 0.05$. Then, $k_0 = \frac{0.05}{0.95} = \frac{1}{19}$. $k_1 = \frac{0.95}{0.05} = 19$. $\alpha = k_0(1-\beta)$ and $\beta = \frac{(1-\alpha)}{k_1}$ subject to $\alpha \le k_0(1-\beta)$ and $\beta \le \frac{(1-\alpha)}{k_1}$.

Example: Consider the following quality control example. We have a sequence of Bernoulli trials. $\theta = P(\text{Failure}) = P(\text{Defective})$. We wish to test sequentially. The rules are 1) reject the lot whenever you find a defective unit, and 2) accept the lot if the first n_0 units are not defective. The hypotheses are $H_0 : \theta = \theta'$ and $H_1 : \theta = \theta'' > \theta'$. N is the number of units inspected at the stopping time. $P(N = n) = (1-\theta)^{n-1}\theta, n = 1, 2, ..., n_0 - 1$.

$$P(N = n_0) = \overbrace{(1-\theta)^{n_0-1}\theta}^{\text{defective}} + \overbrace{(1-\theta)^{n_0-1}(1-\theta)}^{\text{not defective}} = (1-\theta)^{n_0-1},\;\; E(N) = \sum_{n=1}^{n_0-1} n(1-\theta)^{n-1}\theta + n_0(1-\theta)^{n_0-1}.$$

$$1 - \alpha = P(\text{Accept } H_0|H_0) = (1-\theta')^{n_0} \Rightarrow \alpha = 1 - (1-\theta')^{n_0}.$$

14.27 Quadratic Forms

Definition: A homogeneous polynomial of degree two in n variables is called a *quadratic form.*

Example: $x^T A x = \sum_{i,j=1}^n a_{ij} x_i x_j$.

Example: $\sum_{i=1}^n (x_i - \bar{x})^2 = \sum_{i=1}^n x_i^2 - n\bar{x}^2 = x^T I x - x^T \frac{1}{n} I_n I_n^T x$ where

$$I_n = \begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}.$$

$\bar{x} = \frac{x^T I_n}{n} \Rightarrow x^T A x$, $A = I - \frac{1}{n} I_n I_n^T$ and A is an idempotent matrix.

Theorem: Let $x_i, i = 1, 2, ..., n$ be iid random variables with the distribution $N(\mu, \sigma^2), \mu_1 = \mu_2 = \cdots = \mu_n$ as in the text book. And let the scalars be $x^T Ax = x^T A_1 x + \cdots + x^T A_k x$, $Q = Q_1 + Q_2 + \cdots + Q_k$. Let $\frac{Q_1}{\sigma^2}, \frac{Q_2}{\sigma^2}, ..., \frac{Q_{k-1}}{\sigma^2}$ be distributed as chi-squares with $r_1, r_2, ..., r_{k-1}$ degrees of freedom. If Q_k is non-negative, then $Q_k/\sigma^2 \sim \chi^2(r_k)$ where $r_k = r - \sum_{i=1}^{k-1} r_i$.

For the next example, recall that if $y_i \sim N(0, \sigma^2)$ then $\bar{y} \sim N\left(0, \frac{\sigma^2}{n}\right)$.

Example: Suppose that $x_1, x_2, ..., x_n$ are iid random variables with the distribution $N(\mu, \sigma^2)$. We already know that $\sum_{i=1}^n (x_i - \mu)^2 = \sum_{i=1}^n (x_i - \mu)^2 + n(\bar{x} - \mu)^2$. Let $y_i = x_i - \mu$. Then, we have $\sum_{i=1}^n y_i^2 = \sum_{i=1}^n (y_i - \bar{y})^2 + n\bar{y}^2$, $y^T I y = y^T A y + y^T \frac{1}{n} I_n I_n^T y$ where $A = I - \frac{1}{n} I_n I_n^T \Rightarrow Q = Q_1 + Q_2$, $\frac{Q}{\sigma^2} \sim \chi^2(n)$. $\frac{Q_1}{\sigma^2} \sim \chi^2(1) \Rightarrow \frac{Q_2}{\sigma^2} \sim \chi^2(n-1)$ where $\frac{Q_1}{\sigma^2} = \frac{n y^2}{\sigma^2}$ and $\frac{Q_2}{\sigma^2} = \frac{\sum_{i=1}^n (y_i - \bar{y})^2}{\sigma^2} = \frac{\sum_{i=1}^n (x_i - \bar{x})^2}{\sigma^2} \sim \chi^2(n-1)$.

14.28 One-Way ANOVA

Suppose we have the observations

$$\begin{matrix} x_{11} & \cdots & x_{1b} \\ x_{21} & \cdots & x_{2b} \\ \vdots & \vdots & \vdots \\ x_{a1} & \cdots & x_{ab} \end{matrix}$$

where $(x_{11}, ..., x_{1b}) \sim N(\mu_1, \sigma^2)$ to $(x_{a1}, ..., x_{ab}) \sim N(\mu_a, \sigma^2)$. We know from previous courses to use the trick $x_{ij} - \bar{x} = x_{ij} - \bar{x}_{i\cdot} + \bar{x}_{i\cdot} - \bar{x}$. So,

$$ab\, s^2 = \sum_{i,j} (x_{ij} - \bar{x})^2 = \overbrace{\sum (x_{ij} - \bar{x}_{i\cdot})^2}^{Q_1} + \overbrace{b \sum (\bar{x}_{i\cdot} - \bar{x})^2}^{Q_2}.$$

We wish to test the hypothesis $H_0 : \mu_1 = \mu_2 = \cdots = \mu_a$. For the i-th row, $\frac{\sum_{j=1}^b (x_{ij} - \bar{x}_{i\cdot})^2}{b-1}$. Then, $\frac{\sum_{j=1}^b (x_{ij} - \bar{x}_{i\cdot})^2}{\sigma^2} \sim \chi^2(b-1)$ and $\frac{\sum_{i,j} (x_{ij} - \bar{x}_{i\cdot})^2}{\sigma^2} \sim \chi^2[a(b-1)]$. Here, $Q = Q_1 + Q_2$. We can also write

$$\sum (x_{ij} - \bar{x})^2 = \overbrace{\sum (x_{ij} - \bar{x}_{\cdot j})^2}^{Q_3} + \overbrace{a \sum (x_{\cdot j} - \bar{x})^2}^{Q_4}.$$

Here, $Q = Q_3 + Q_4$. We can also write

$$\sum (x_{ij} - \bar{x})^2 = \sum (x_{ij} - \bar{x}_{i\cdot} + \bar{x}_{\cdot j} + \bar{x})^2 + \overbrace{b \sum (\bar{x}_i - \bar{x})^2}^{Q_2} + \overbrace{a \sum (\bar{x}_{\cdot j} - \bar{x})^2}^{Q_4},$$

Here, $Q = Q_5 + Q_2 + Q_4$.

14.28.1 General Result (Normal Distribution)

Consider the likelihood function

$$L = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-\frac{1}{2\sigma^2} Q(\underline{x}, \underline{\theta})}.$$

Let $\underline{\widehat{\theta}}$ be the mle of $\underline{\theta}$. The mle of σ^2 is $\widehat{\sigma}^2 = \frac{Q(\underline{x},\underline{\widehat{\theta}})}{n}$. Look at

$$L(\widehat{\theta}, \widehat{\sigma}|\underline{x}) = \overbrace{\frac{e^{-\frac{n}{2}}}{(2\pi)^{n/2}}}^{\text{Constant}} \times \frac{1}{\widehat{\sigma}^n}.$$

This is the likelihood function of any hypothesis. In the One-Way ANOVA, $x_{ij} \sim N(\mu_i, \theta), i = 1, 2, ..., a; j = 1, 2, ..., b$. $H_0 : \mu_1 = \mu_2 = \cdots = \mu_a = \mu$. Under $\Omega, \widehat{\mu}_i = \bar{x}_{i\cdot}$ and $\widehat{\theta}_\Omega = \frac{\sum(x_{ij}-\bar{x}_{i\cdot})^2}{n}$.

$$L(\widehat{\mu}_i, \widehat{\theta}_\Omega) = \frac{e^{-\frac{n}{2}}}{(2\pi)^{n/2}} \times \frac{1}{(\widehat{\theta}_\Omega)^{n/2}}.$$

The alternative sample space W gives $\widehat{\mu} = \bar{x}$ and $\widehat{\theta}_W = \frac{\sum(x_{ij}-\bar{x})^2}{n}$. The likelihood function is

$$L(\widehat{\mu}_i, \widehat{\theta}_W) = \frac{e^{-\frac{n}{2}}}{(2\pi)^{n/2}} \times \frac{1}{(\widehat{\theta}_W)^{n/2}}.$$

Then, the likelihood ratio for the test is

$$\lambda = \frac{L(\widehat{\theta}_W)}{L(\widehat{\theta}_\Omega)} = \left(\frac{\widehat{\theta}_\Omega}{\widehat{\theta}_W}\right)^{n/2} = \left(\frac{\sum(x_{ij}-\bar{x}_{i\cdot})^2}{\sum(x_{ij}-\bar{x})^2}\right)^{n/2} \leq \lambda_0 \Rightarrow \frac{\sum(x_{ij}-\bar{x})^2}{\sum(x_{ij}-\bar{x}_{i\cdot})^2} \geq c \Rightarrow \frac{Q_1+Q_2}{Q_1} \geq c \Rightarrow \frac{Q_2}{Q_1} \geq c-1.$$

Under $H_0 : \frac{Q_2}{\theta} \sim \chi^2(a-1)$ and $\frac{Q_1}{\theta} \sim \chi^2[a(b-1)]$.

$$F = \frac{\frac{Q_2}{a-1}}{\frac{Q_1}{a(b-1)}} \geq F^* \text{ from the tables.}$$

F is distributed with $a-1$ and $a(b-1)$ degrees of freedom. Thus,

$$F = \frac{a(b-1)}{a-1}\frac{b\sum(\bar{x}_{i\cdot}-\bar{x})^2}{\sum(x_{ij}-\bar{x}_{i\cdot})^2}$$

Lecture 20 on May 6, 1998 is missing.

14.29 Homework and Answers

Most of these answers came from Siriluck Jermyitpornchri since the answers are in her handwriting.

8.2 let $x_1, x_2, ..., x_n$ denote a random sample from a distribution that is $N(\theta, \sigma^2)$, $-\infty < \theta < \infty$, where σ^2 is a given positive number. Let $y = \bar{x}$, the mean of the random sample. Take the loss function to be $\mathrm{L}[\theta, \delta(y)] = |\theta - \delta(y)|$. If θ is an observed value of the random variable Θ, that is $N(\mu, \tau^2)$, where $\tau^2 > 0$ and μ are known numbers, find the Baye's solution $\delta(y)$ for a point estimate of θ.

Solution: We know that $y \sim N(\theta, \sigma^2), -\infty < \theta < \infty$ where σ^2 is a given positive number. Therefore, $y = \bar{x} \sim N\left(\theta, \frac{\sigma^2}{n}\right)$ and $\bar{x}$ is sufficient for θ. Therefore,

$$g(y|\theta) = \left(2n\frac{\sigma^2}{n}\right)^{-1/2} e^{-\frac{n}{2\sigma^2}(y-\theta)^2} = R_1 e^{-\frac{n}{2\sigma^2}(y-\theta)^2}, -\infty < y < \infty.$$

Therefore, $\Theta \sim N(\mu, \tau^2)$, where $\tau^2 > 0$ and μ are know numbers. Therefore, $h(\theta) = (2\pi\tau^2)^{-1/2}$ $e^{-\frac{1}{2\tau^2}(\theta-\mu)^2} = R_2\ e^{-\frac{1}{2\tau^2}(\theta-\mu)^2}$, $-\infty < \theta < \infty$. From Chapter 4 in the text book, we know that $(\theta, \bar{x})$ has a bivariate normal distribution with means $\mu_1 = \mu$ and $\mu_2 = \theta$. Also, $\sigma_1^2 = Var(\theta) = \tau^2$ and $\sigma_2^2 = Var(y)\frac{\sigma_2^2}{n}$ and $\rho = Cov(\theta, \bar{x})$. Therefore, $\theta|y \sim N\left(\mu_1 + \rho\frac{\sigma_1}{\sigma_2}(y-\theta), \sigma_1^2(1-\rho^2)\right)$. Note that $Cov(\underline{\mu}, \underline{\bar{x}}) = Cov(\underline{\mu}, \frac{1}{n}J\underline{\mu}) = Var(\underline{\mu})\frac{1}{n}J'$ where the i-th element is $Cov(x_i, \bar{x}) = Var(x_i)\frac{1}{n}$.

$$k(\theta|y) \propto \exp\left\{-\frac{n}{2\sigma^2}\left(y^2 - 2y\theta + \theta^2\right) + \frac{1}{2\tau}\left(\theta^2 - 2\theta\mu + \mu^2\right)\right\} \propto \exp\left\{-\frac{1}{2}\left(\theta - \frac{yn\tau^2 + \mu\sigma^2}{n\tau^2 + \sigma^2}\right)^2\right\} \Rightarrow$$

$$k(\theta|y) \sim \text{ Normal and } E(\theta|y) = \frac{yn\tau^2 + \mu\sigma^2}{n\tau^2 + \sigma^2} \Rightarrow \text{Ł}[\theta, \delta(y)] = [\theta - \delta(y)] \Rightarrow R[\delta(y)] = E_{\theta|y}|\theta - \delta(y)|.$$

For what $\delta(y)$ is R the minimum? It is the minimum if $\delta(y)$ is the mle of $\theta|y$. Therefore, $\int_{-\infty}^{\delta(y)} k(\theta|y)\, d\theta = \int_{\delta(y)}^{\infty} k(\theta|y)\, d\theta = \frac{1}{2}$. In this case, we know that

$$\frac{1}{2} = \int_0^{E(\theta|y)} k(\theta|y)\, dy, \;\; \frac{1}{2} = \Phi[E(\theta|y)], \;\; \frac{1}{2} = \Phi\left[\frac{yn\tau^2 + \mu\sigma^2}{n\tau^2 + \sigma^2}\right] = \Phi\left[\frac{y\tau^2 + \mu\frac{\sigma^2}{n}}{\tau^2 + \frac{\sigma^2}{n}}\right].$$

Therefore,

$$\delta(y) = \frac{y\tau^2 + \mu\frac{\sigma^2}{n}}{\left(\tau^2 + \frac{\sigma^2}{n}\right)}.$$

8.15 Let x have a gamma distribution with $\alpha = 4$ and $\beta = \theta > 0$.

a. Find the Fisher information $I(\theta)$. Solution: $x \sim Gamma(4, \theta)$. Then,

$$f(x|\theta) = \frac{1}{\Gamma(4)\theta^4}x^3 e^{-\frac{x}{\theta}}, x > 0.$$

We know that $E(x) = 4\theta$ and $Var(x) = 4\theta^2$.

$$\log f(x|\theta) = -\log\Gamma(4) - 4\log\theta + 3\log x - \frac{x}{\theta}, \;\; \frac{d\log f(x|\theta)}{d\theta} = -\frac{4}{\theta} + \frac{x}{\theta^2} = \frac{1}{\theta^2}\left[x - 4\theta\right].$$

$$I(\theta) = E\left(\frac{d\log f}{d\theta}\right)^2 = E\left(\frac{1}{\theta^2}\left[x - 4\theta\right]\right)^2 = \frac{1}{\theta^4}E(x-4\theta)^2 = \frac{1}{\theta^4}Var(x) = \frac{1}{\theta^4}4\theta^2 = \frac{4}{\theta^2}.$$

b. If $x_1, x_2, ..., x_n$ is a random sample from this distribution, show that the mle of θ is an efficient estimator of θ. Solution: The likelihood function of θ is $L(\theta|\underline{x}) = \prod_{i=1}^{n} f(x_i|\theta) = \frac{1}{\Gamma(4)^n \theta^{4n}} e^{-\frac{n\bar{x}}{\theta}} \prod_{i=1}^{n} x_i^3$, $\log L(\theta|\underline{x}) = -n \log \Gamma(4) - 4n \log \theta - n\frac{\bar{x}}{\theta} + \sum_{i=1}^{n} \log x_i^3$, $\frac{d}{d\theta} \log L(\theta|\underline{x}) = -\frac{4n}{\theta} + \frac{n\bar{x}}{\theta^2} = 0 \Rightarrow \frac{n\bar{x}}{\theta^2} = \frac{4n}{\theta} \Rightarrow \theta = \frac{\bar{x}}{4}$. So, $\widehat{\theta} = \frac{\bar{x}}{4}$ is the mle of θ. Consider

$$E\left(\frac{\bar{x}}{4}\right) = \frac{1}{4} E\left(\sum_{i=1}^{n} \frac{x_i}{n}\right) = \frac{1}{4} n4\theta = \theta.$$

Thus, $\frac{\bar{x}}{4}$ is an unbiased estimator of θ and

$$Var\left(\frac{\bar{x}}{4}\right) = \frac{1}{16} Var\left(\sum_{i=1}^{n} \frac{x_i}{n}\right) = \frac{1}{16n^2} Var\left(\sum_{i=1}^{n} x_i\right) = \frac{1}{16n^2} n4\theta^2 = \frac{\theta^2}{4n}.$$

Consider the efficiency of

$$\frac{\bar{x}}{4} = \frac{\frac{1}{nI(\theta)}}{Var\left(\frac{\bar{x}}{4}\right)} = \frac{\frac{1}{n\frac{4}{\theta^2}}}{\frac{\theta^2}{4n}} = 1.$$

Thus, $\widehat{\theta} = \frac{\bar{x}}{4}$ is an efficient estimator of θ.

8.19 Let $(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)$ be a random sample from a bivariate normal distribution with unknown mean θ_1 and θ_2 and with known variances and correlation coefficient σ_1^2, σ_2^2, and ρ respectively. Find the maximum likelihood estimators $\widehat{\theta}_1$ and $\widehat{\theta}_2$ of θ_1 and θ_2 and their approximate variance-covariance matrix. In this case, does the latter provide the exact variances and covariances?

The variance and covariance matrices are as follow.

$$\left.\begin{array}{l} \frac{d \log L}{d\theta_1} = 0 \Rightarrow (\bar{x} - \theta_1) = \rho\frac{\sigma_1}{\sigma_2}(\bar{y} - \theta_2) \\ \\ \frac{d \log L}{d\theta_2} = 0 \Rightarrow (\bar{y} - \theta_2) = \rho\frac{\sigma_2}{\sigma_1}(\bar{x} - \theta_1) \end{array}\right\}$$

$(\bar{y} - \theta_2) = \rho^2(\bar{y} - \theta_2) \Rightarrow (\bar{y} - \theta_2)(1 - \rho^2) = 0, \rho^2 \neq 1 \Rightarrow \bar{y} - \theta_2 = 0 \Rightarrow \widehat{\theta}_2 = \bar{y}$. Similarly, $\widehat{\theta}_1 = \bar{x}, Var(\widehat{\theta}_1) = \frac{\sigma_1^2}{n}, Var(\widehat{\theta}_2) = \frac{\sigma_2^2}{n}$ $Cov(\widehat{\theta}_1, \widehat{\theta}_2) = Cov\left(\sum \frac{x_i}{n}, \sum \frac{y_i}{n}\right) = \sum \left(\frac{1}{n} \times \frac{1}{n}\right) Cov(x_i, y_i) = \frac{Cov(x_i, y_i)}{n} = \frac{\rho\sigma_1\sigma_2}{n}$.

$$\frac{I^{-1}(\theta)}{n} = \begin{pmatrix} \frac{\sigma_1^2}{n} & \frac{\rho\sigma_1\sigma_2}{n} \\ \frac{\rho\sigma_1\sigma_2}{n} & \frac{\sigma_2^2}{n} \end{pmatrix}$$

$Q = \sum_{i=1}^{n} \frac{(x_i - \theta_1)^2}{\sigma_1^2} - 2\rho \sum_{i=1}^{n} \frac{(x_i - \theta_1)(y_i - \theta_2)}{\sigma_1\sigma_2} + \sum_{i=1}^{n} \frac{(y_i - \theta_2)^2}{\sigma_2^2}$, $\frac{dQ}{d\theta_1} = 0 \Rightarrow \bar{x} - \theta_1 = \rho\frac{\sigma_1}{\sigma_2}(\bar{y} - \theta_2)$ $\frac{dQ}{d\theta_2} = 0 \Rightarrow \bar{y} - \theta_2 = \rho\frac{\sigma_1}{\sigma_2}(\bar{x} - \theta_1) \Rightarrow (\bar{y} - \theta_2) = \rho^2(\bar{y} - \theta_2) \Rightarrow (\bar{y} - \theta_2)(1 - \rho^2) = 0$.

8.28 Let $x_1, x_2, ..., x_n$ be a random sample from a distribution with the pdf

$$f(x, \theta) = \begin{cases} \frac{\theta}{(1+x)^{\theta+1}}, & 0 < x < \infty; \theta > 0. \\ 0, & \text{otherwise.} \end{cases}$$

a. Find the mle $\widehat{\theta}$ of θ and argue that it is a complete sufficient statistic for θ. Is $\widehat{\theta}$ unbiased? Solution: The likelihood function of θ is

$$L(\theta|\underline{x}) = \prod_{i=1}^{n} \frac{\theta}{(1+x_i)^{\theta+1}} = \theta^n \prod_{i=1}^{n} \frac{1}{(1+x_i)^{\theta+1}}, \ \ \log L(\theta|\underline{x}) = n\log\theta - (\theta+1)\sum_{i=1}^{n}\log(1+x_i),$$

$$\frac{d}{d\theta}\log L(\theta|\underline{x}) = \frac{n}{\theta} - \sum_{i=1}^{n}\log(1+x_i) = 0 \Rightarrow \frac{1}{\theta} = \frac{1}{n}\sum_{i=1}^{n}\log(1+x_i)$$

which is the mle of $\frac{1}{\theta}$. $\widehat{\theta} = \frac{n}{\sum_{i=1}^{n}\log(1+x_i)}$ is the mle of θ. Consider $f(x|\theta) = e^{-(\theta+1)\log(1+x)+\log\theta}$. This is in the exponential family. Therefore $\sum_{i=1}^{n}\log(1+x_i)$ is a complete sufficient statistic for θ. Therefore, $\frac{n}{\sum_{i=1}^{n}\log(1+x_i)}$ is a complete sufficient statistic for θ. Unfortunately, $\widehat{\theta}$ is biased for θ. The proof has been omitted.

b. If $\widehat{\theta}$ is adjusted so that it is an unbiased estimator of θ, what is a lower bound for the variance of this unbiased estimator? Solution: $\widehat{\theta}$ can be adjusted so that it is unbiased. Let T^* be an unbiased estimator for θ. Then, find $I(\theta)$. $f(x|\theta)\,dx = \frac{\theta}{(1+x)^{\theta+1}}\,dx, 0 < x < \infty$, $y = \log(1+x) \Rightarrow 1+x = e^y$, $dx = e^y\,dy$ $f(x|\theta)\,dx = \frac{\theta}{e^{(\theta+1)y}}e^y\,dy = \theta e^{-\theta y}\,dy \Rightarrow y = \log(1+x) \sim Exp(\theta)$. $\widehat{\theta} = \frac{n}{\sum\log(1+x_i)} = \frac{n}{\sum y_i}$, $\sum y_i \sim Gamma(n,\theta)$. $U = \sum y_i \sim Gamma(n,\theta)$. $E\left(\frac{1}{U}\right) = \int_0^\infty \frac{e^n e^{-\theta U}U^{n-1}}{\sqrt{n}}\frac{1}{U}dU = \frac{\theta}{n-1}$ $E(\widehat{\theta}) = nE\left(\frac{1}{\sum y_i}\right) = \frac{n}{n-1}\theta$. $\tilde{\theta} = \frac{n-1}{n}\widehat{\theta}$ is unbiased. $Var(\tilde{\theta}) = \frac{1}{nI(\theta)}$, where $\frac{1}{nI(\theta)} = \frac{\theta^2}{n}$.

9.10 Let $x_1, x_2, ..., x_{10}$ denote a random sample of size 10 from a Poisson distribution with mean θ. Show that the critical region C defined by $\sum_{i=1}^{10} x_i \geq 3$ is a best critical region for testing $H_0 : \theta = 0.1$ against $H_1 : \theta = 0.5$. Determine, for this test, the significance level α and the power at $\theta = 0.5$. Solution: We reject H_0 if $\sum_{i=1}^{10} x_i \geq 3$. Let $y = \sum_{i=1}^{10} x_i \Rightarrow y \sim Poisson(10,\theta)$. Consider that it is proportional to

$$P(\underline{x}\in C|H_0) = P\left(\sum_{i=1}^{10} x_i \geq 3 \middle| \theta = 0.1\right) = P\left(y \geq 3|\theta = 0.1\right) = \sum_{y=3}^{10}\frac{e^{-1}1^y}{y!} = 1 - 0.920 = 0.08.$$

and consider the power $1-\beta$ as

$$1-\beta = P(\underline{x}\in C|H_1) = P(y\geq 3|\theta = 0.5) = \sum_{i=3}^{10}\frac{e^{-5}5^y}{y!} = 1 - 0.125 = 0.875.$$

For this test, the significance level α and the power at $\theta = 0.5$ are 0.08 and 0.875 respectively. A likelihood function of θ is

$$L(\theta|\underline{x}) = \prod_{i=1}^{n}\frac{e^{-\theta}\theta^{x_i}}{x_i!} = \frac{e^{-n\theta}\theta^{\sum_{i=1}^{n}x_i}}{\prod_{i=1}^{n}x_i!} = \frac{e^{-10\theta}\theta^{\sum_{i=1}^{10}x_i}}{\prod_{i=1}^{10}x_i!}.$$

$$\frac{L(\theta_0|\underline{x})}{L(\theta_1|\underline{x})} = \frac{e^{-1}(0.1)^{\sum_{i=1}^{10}x_i}}{\prod_{i=1}^{10}x_i!} \times \frac{\prod_{i=1}^{10}x_i!}{e^{-5}(0.5)^{\sum_{i=1}^{10}x_i}} \leq k,$$

$$\frac{e^4}{5^{\sum_{i=1}^{10}x_i}} \leq k \Rightarrow 5^{\sum_{i=1}^{10}x_i} \geq \frac{e^4}{k} = k_1 \Rightarrow \sum_{i=1}^{10}x_i\log 5 \geq \log k_1 = k_2 \Rightarrow \sum_{i=1}^{10}x_i \geq \frac{k_2}{\log 5} = k_3.$$

Therefore, the critical region for this test is $\sum_{i=1}^{10} x_i \geq k_3$. Let $\sum_{i=1}^{10} x_i \geq 3 \Rightarrow k_3 = 3$. Then,

$$k_3 = \frac{k_2}{\log 5} \Rightarrow k_2 = 3\log 5 \Rightarrow k_2 = \log k_1 \Rightarrow e^{k_2} = k_1 \Rightarrow k_1 = e^{3\log 5} \Rightarrow k_1 = \frac{e^4}{k} \Rightarrow k = \frac{e^4}{e^{3\log 5}} = \frac{e^4}{15} \Rightarrow$$

$$\frac{L(\theta_0|\underline{x})}{L(\theta_1|\underline{x})} = \frac{e^4}{5^{\sum_{i=1}^{10}}} \leq \frac{e^4}{15} = k.$$

Thus, the critical region C defined by $\sum_{i=1}^{10} x_i \geq 3$ is the best critical region for testing $H_0 : \theta = 0.1$ against $H_1 : \theta = 0.5$.

9.12 Let x have a pdf of the form $f(x,\theta) = \frac{1}{\theta}, 0 < x < \theta$ and zero elsewhere. Let $y_1 < y_2 < y_3 < y_4$ denote the order statistics of a random sample of size 4 from this distribution. We reject $H_0 : \theta = 1$ and accept $H_1 : \theta \neq 1$ if either $y_4 \leq \frac{1}{2}$ or $y_4 \geq 1$. Find the power function $K(\theta), 0 < \theta$ of the test. The cdf of x is

$$F(x,\theta) = \begin{cases} 0, & x \leq 0. \\ \frac{x}{\theta}, & 0 < x < \theta. \\ 1, & x \geq \theta. \end{cases}$$

Find the pdf of y_4. $f_4(y_4) = 4[F(y_4)]^{4-1} f(y_4)$, $0 < y_4 < \theta$,

$$\frac{4y_4^3}{\theta^3}\frac{1}{\theta} = \begin{cases} \frac{4y_4^3}{\theta^4}, & 0 < y_4 < \theta. \\ 0, & \text{otherwise}. \end{cases}$$

The statistical power is given by $k(\theta) = P(\text{Reject } H_0|H_1), \theta > 0$. Consider

$$0 < \theta \leq \frac{1}{2} \Rightarrow 0 < y_4 < \theta \leq \frac{1}{2} \Rightarrow y_4 \leq \frac{1}{2},\ \ k(\theta) = \int_0^\theta \frac{4y_4^3}{\theta^4}\,dy_4 = \frac{y_4^4}{\theta^4} = 1.$$

Consider

$$\frac{1}{2} < \theta < 1 \Rightarrow 0 < y_4 < \frac{1}{2} < \theta < 1 \Rightarrow y_4 \leq \frac{1}{2},\ \ k(\theta) = \int_0^{\frac{1}{2}} \frac{4y_4^3}{\theta^4}\,dy_4 = \left.\frac{y_4^4}{\theta^4}\right|_0^{\frac{1}{2}} = \frac{1}{16\theta^4}.$$

Consider

$$\theta \geq 1 \Rightarrow 1 \leq y_4 < \theta \text{ or } 0 < y_4 \leq \frac{1}{2} < 1 \leq \theta \Rightarrow y_4 \leq \frac{1}{2}.$$

Then,

$$k(\theta) = k(\theta) = \int_\theta^1 \frac{4y_4^3}{\theta^4}\,dy_4 + \int_0^{\frac{1}{2}} \frac{4y_4^3}{\theta^4}\,dy_4 = \left.\frac{y_4^4}{\theta^4}\right|_\theta^1 + \frac{1}{16\theta^4} = \left(1 - \frac{1}{\theta^4}\right) + \frac{1}{16\theta^4} = 1 - \frac{15}{16\theta^4}.$$

The power function of this test is

$$k(\theta) = \begin{cases} 1, & 0 < \theta \leq \frac{1}{2}. \\ \frac{1}{16\theta^4}, & \frac{1}{2} < \theta < 1. \\ 1 - \frac{15}{16\theta^4}, & \theta \geq 1. \end{cases}$$

9.22 Let x have the pdf $f(x,\theta)=\theta^x(1-\theta)^{1-x}, x=0,1$ and zero elsewhere. We test $H_0:\theta=\frac{1}{2}$ against $H_1:\theta<\frac{1}{2}$. by taking a random sample $x_1,x_2,...,x_5$ of size 5 and rejecting H_0 if $y=\sum_{i=1}^5 x_i$ is observed to be less-than or equal to a constant k.

a. Show that this is a uniformly most powerful test. Solution: We are testing $H_0:\theta=\frac{1}{2}$ against $H_1:\theta<\frac{1}{2}$. We reject H_0 if $y=\sum_{i=1}^5 x_i\le k$. $x\sim Bernoulli(\theta)$. The likelihood function of θ is

$$L(\theta|\underline{x})=\prod_{i=1}^{5}\theta^{x_i}(1-\theta)^{1-x_i}=\theta^{\sum_{i=1}^5 x_i}(1-\theta)^{5-\sum_{i=1}^5 x_i}.$$

Consider

$$\frac{L(\theta_0|\underline{x})}{L(\theta_1|\underline{x})}=\frac{\theta_0^{\sum_{i=1}^5 x_i}(1-\theta_0)^{5-\sum_{i=1}^5 x_i}}{\theta_1^{\sum_{i=1}^5 x_i}(1-\theta_1)^{5-\sum_{i=1}^5 x_i}}\le k,\ \left[\frac{\theta_0(1-\theta_1)}{\theta_1(1-\theta_0)}\right]^{\sum_{i=1}^5 x_i}\left[\frac{1-\theta_0}{1-\theta_1}\right]^5\le k,$$

$$\left[\frac{\theta_0(1-\theta_1)}{\theta_1(1-\theta_0)}\right]^{\sum_{i=1}^5 x_i}\le k\left[\frac{1-\theta_1}{1-\theta_0}\right]^5=k_1,\ \sum_{i=1}^{5}x_i\log\frac{\theta_0(1-\theta_1)}{\theta_1(1-\theta_0)}\le\log k_1=k_2,$$

$$\sum_{i=1}^{5}x_i\le\frac{k_2}{\log\frac{\theta_0(1-\theta_1)}{\theta_1(1-\theta_0)}}=k\Rightarrow\theta_0=\frac{1}{2}\text{ and }\theta_1<\frac{1}{2}\Rightarrow\frac{\theta_0}{\theta_1}>1,\frac{(1-\theta_1)}{(1-\theta_0)}>1\text{ and }\frac{\theta_0(1-\theta_1)}{\theta_1(1-\theta_0)}>1.$$

Therefore, the best critical region does not depend on θ_1. Therefore, this test is a uniformly most powerful test.

b. Find the significance level when $k=1$. Solution: Consider $\alpha=P(\text{Reject }H_0|H_0)$ when $k=1$.

$$\alpha=P\left(\sum_{i=1}^5 x_i\le 1\middle|\frac{1}{2}\right)=\sum_{y=0}^{5}\binom{5}{y}\left(\frac{1}{2}\right)^y\left(\frac{1}{2}\right)^{5-y}=\left(\frac{1}{2}\right)^5+5\left(\frac{1}{2}\right)^5=0.1875.$$

The significance level is 0.1875 when $k=1$.

c. Find the significance level when $k=0$. Solution: Consider $\alpha=P(\text{Reject }H_0|H_0)$ when $k=0$.

$$\alpha=P\left(\sum_{i=1}^5 x_i\le 0\middle|\frac{1}{2}\right)=\binom{5}{0}\left(\frac{1}{2}\right)^0\left(\frac{1}{2}\right)^5=0.03125$$

The significance level is 0.03125 when $k=0$.

d. By using a randomized test, modify the tests given in parts (b) and (c) to find a test with significance level $\alpha=\frac{2}{32}$. Solution: Consider

$$\alpha=P\left(\sum_{i=1}^5 x_i\le 0\right)+\alpha_3 P\left(\sum_{i=1}^5 x_i=1\right),\ \frac{2}{e^5}=\frac{1}{2^5}+\alpha_3\frac{5}{e^5}\Rightarrow\alpha_3=\frac{1}{2^5}\times\frac{2^5}{5}=\frac{1}{5}\Rightarrow\alpha_3=\frac{1}{5}.$$

Then, the randomized test is

$$\Phi(x_1, x_2, ..., x_5) = \begin{cases} 1, & \text{if } \sum_{i=1}^{5} x_i < 1. \\ \frac{1}{5}, & \sum_{i=1}^{5} = 1. \\ 0, & \sum_{i=1}^{5} x_i > 1. \end{cases}$$

with a significance level of $\alpha = \frac{2}{32}$.

9.30 Let $x_1, x_2, ..., x_n$ and $y_1, y_2, ..., y_m$ be independent random samples from the distributions $N(\theta_1, \theta_3)$ and $N(\theta_2, \theta_4)$, respectfully. Show that the likelihood ratio for testing $H_0 : \theta_1 = \theta_2, \theta_3 = \theta_4$ against all alternatives is given by

$$\frac{\left[\sum_{i=1}^{n}(x_i - \bar{x})^2 \Big/ n\right]^{n/2} \left[\sum_{i=1}^{m}(y_i - \bar{y})^2 \Big/ m\right]^{m/2}}{\left\{\left[\sum_{i=1}^{n}(x_i - \mu)^2 + \sum_{i=1}^{m}(y_i - \mu)^2\right] \Big/ (n + m)\right\}^{\frac{n+m}{2}}}$$

where $\mu = \frac{n\bar{x}+m\bar{y}}{n+m}$. Define the sample spaces $W = \{(\theta_1, \theta_2, \theta_3, \theta_4); -\infty < \theta_1 = \theta_2 < \infty, 0 < \theta_3 = \theta_4 < \infty\}$ and $\Omega = \{(\theta_1, \theta_2, \theta_3, \theta_4); -\infty < \theta_1 < \infty, -\infty < \theta_2 < \infty, 0 < \theta_3 < \infty, 0 < \theta_4 < \infty\}$. Since $x_1, x_2, ..., x_n$ and $y_1, y_2, ..., y_m$ are independent random samples, then

$$L(\theta|\underline{xy}) = \left[\left(\frac{1}{2\pi\theta_3}\right)^{n/2} e^{-\frac{1}{2\theta_3}\sum_{i=1}^{n}(x_i-\theta_1)^2}\right]\left[\left(\frac{1}{2\pi\theta_4}\right)^{m/2} e^{-\frac{1}{2\theta_4}\sum_{i=1}^{m}(y_i-\theta_2)^2}\right] =$$

$$\left(\frac{1}{2\pi}\right)^{\frac{n+m}{2}} \frac{1}{\theta_3^{n/2}\theta_4^{m/2}} e^{-\frac{1}{2\theta_3}\sum_{i=1}^{n}(x_i-\theta_1)^2 - \frac{1}{2\theta_4}\sum_{i=1}^{m}(y_i-\theta_2)^2}.$$

Under W

$$L(\theta_W|\underline{x}, \underline{y}) = \left(\frac{1}{2\pi\theta_3}\right)^{\frac{n+m}{2}} e^{-\frac{1}{2\theta_3}\left\{\sum_{j=1}^{n}(x_j-\theta_1)^2 + \sum_{j=1}^{m}(y_j-\theta_2)^2\right\}}.$$

Consider,

$$\log L(\theta_W|\underline{x}, \underline{y}) = -\frac{n+m}{2}\log 2\pi\theta_3 - \frac{1}{2\theta_3}\sum_{j=1}^{n}(x_j - \theta_1)^2 - \frac{1}{2\theta_3}\sum_{j=1}^{m}(y_j - \theta_2)^2 =$$

$$-\frac{n+m}{2}\log 2\pi\theta_3 - \frac{1}{2\theta_3}\left(\sum_{j=1}^{n} x_j^2 - 2\theta_1\sum_{j=1}^{n} x_j + n\theta_1^2\right) - \frac{1}{2\theta_3}\left(\sum_{j=1}^{m} y_j^2 - 2\theta_1\sum_{j=1}^{n} y_j + m\theta_1^2\right).$$

$$\frac{d}{d\theta_1}\log L(\theta_W|\underline{x},\underline{y}) = -\frac{1}{2\theta_3}\left(2\sum_{i=1}^{n}x_i + 2n\theta_1\right) - \frac{1}{2\theta_3}\left(2\sum_{j=1}^{m}y_j + 2m\theta_1\right) = 0 \Rightarrow$$

$$\sum_{i=1}^{n}x_i + \sum_{j=1}^{m}y_j - (n+m)\theta_1 = 0 \Rightarrow \theta_1 = \frac{\sum_{i=1}^{n}x_i + \sum_{j=1}^{m}y_j}{(n+m)} = \frac{n\bar{x}+m\bar{y}}{n+m}.$$

So, the mle of θ is

$$\widehat{\theta}_1 = \frac{\sum_{i=1}^{n}x_i + \sum_{j=1}^{m}y_j}{(n+m)} = \frac{n\bar{x}+m\bar{y}}{n+m}.$$

$$\frac{d}{d\theta_3}\log L(\theta_W|\underline{x},\underline{y}) = -\frac{n+m}{2}\frac{1}{2\pi\theta_3}2\pi + \frac{\sum_{i=1}^{n}(x_i-\theta_1)^2}{2\theta_3^2} + \frac{\sum_{j=1}^{m}(y_j-\theta_2)^2}{2\theta_3^2} = 0 \Rightarrow$$

$$\sum_{i=1}^{n}(x_i-\theta_1)^2 + \sum_{j=1}^{m}(y_j-\theta_2)^2 - (n+m)\theta_3 = 0 \Rightarrow \theta_3 = \frac{\sum_{i=1}^{n}(x_i-\theta_1)^2 + \sum_{j=1}^{m}(y_j-\theta_2)^2}{n+m} \Rightarrow$$

$$\widehat{\theta}_3 = \frac{\sum_{i=1}^{n}(x_i-\widehat{\theta}_1)^2 + \sum_{j=1}^{m}(y_j-\widehat{\theta}_2)^2}{n+m}.$$

Therefore,

$$\widehat{\theta}_3 = \frac{\sum_{i=1}^{n}(x_i-\widehat{\theta}_1)^2 + \sum_{j=1}^{m}(y_j-\widehat{\theta}_2)^2}{n+m}$$

is the mle of θ_3. Therefore,

$$L(\widehat{\theta}_W|\underline{x},\underline{y}) = \left(\frac{1}{2\pi\widehat{\theta}_3}\right)^{\frac{n+m}{2}} e^{-\frac{(n+m)}{2}}.$$

Under Ω

$$L(\widehat{\theta}_W|\underline{x},\underline{y}) = \left(\frac{1}{2\pi}\right)^{\frac{n+m}{2}} \frac{1}{\theta_3^{\frac{n}{2}}\theta_4^{\frac{m}{2}}} \exp\left\{-\frac{1}{2\theta_3}\sum_{i=1}^{n}(x_i-\theta_1)^2 - \frac{1}{2\theta_4}\sum_{j=1}^{m}(y_i-\theta_2)^2\right\}.$$

Consider,

$$\log L(\widehat{\theta}_\Omega|\underline{x},\underline{y}) = -\frac{n+m}{2}\log 2\pi - \frac{n}{2}\log\theta_3 - \frac{m}{2}\log\theta_4 - \frac{1}{2\theta_3}\sum_{i=1}^{n}(x_i-\theta_1)^2 - \frac{1}{2\theta_4}\sum_{j=1}^{m}(y_j-\theta_2)^2.$$

$$\frac{d}{d\theta_1}\log L(\widehat{\theta}_\Omega|\underline{x},\underline{y}) = -\frac{1}{2\theta_3}2\sum_{i=1}^{n}(x_i-\theta_1)(-1) = 0 \Rightarrow \sum_{i=1}^{n}(x_i-\theta_1) = 0 \Rightarrow \theta_1 = \bar{x}.$$

$$\frac{d}{d\theta_2}\log L(\widehat{\theta}_\Omega|\underline{x},\underline{y}) = -\frac{1}{2\theta_4}2\sum_{j=1}^{m}(y_j-\theta_2)(-1) = 0 \Rightarrow \theta_2 = \bar{y}.$$

$$\frac{d}{d\theta_3}\log L(\widehat{\theta}_\Omega|\underline{x},\underline{y}) = -\frac{n}{2\theta_3}+\frac{1}{2\theta_3^2}\sum_{i=1}^{n}(x_i-\theta_1)^2 = 0 \Rightarrow \theta_3 = \frac{\sum_{i=1}^{n}(x_i-\theta_1)^2}{n}.$$

$$\frac{d}{d\theta_4}\log L(\widehat{\theta}_\Omega|\underline{x},\underline{y}) = -\frac{n}{2\theta_4}+\frac{1}{2\theta_4^2}\sum_{j=1}^{m}(y_j-\theta_2)^2 = 0 \Rightarrow \theta_4 = \frac{\sum_{j=1}^{m}(y_j-\theta_2)^2}{m}.$$

Therefore,

$$L(\widehat{\theta}_\Omega|\underline{x},\underline{y}) = \left(\frac{1}{2\pi}\right)^{\frac{n+m}{2}}\frac{1}{\left(\widehat{\theta}_3\right)^{n/2}\left(\widehat{\theta}_4\right)^{m/2}}e^{-\frac{n+m}{2}}.$$

Consider

$$\lambda = \frac{L(\widehat{\theta}_W|\underline{x},\underline{y})}{L(\widehat{\theta}_\Omega|\underline{x},\underline{y})} = \frac{\left(\frac{1}{2\pi}\right)^{\frac{n+m}{2}}\frac{(n+m)^{\frac{n+m}{2}}}{\left[\sum_{i=1}^{n}\left(x_i-\frac{n\bar{x}+m\bar{y}}{n+m}\right)^2+\sum_{j=1}^{m}\left(y_j-\frac{n\bar{y}+m\bar{y}}{n+m}\right)^2\right]^{\frac{n+m}{2}}}e^{-\frac{n+m}{2}}}{\left(\frac{1}{2\pi}\right)^{\frac{n+m}{2}}\frac{1}{\left[\sum_{i=1}^{n}\frac{(x_i-\bar{x})^2}{n}\right]^{\frac{n}{2}}\left[\sum_{j=1}^{m}\frac{(y_j-\bar{y})^2}{m}\right]^{\frac{m}{2}}}e^{-\frac{n+m}{2}}} =$$

$$\frac{\left[\sum_{i=1}^{n}\frac{(x_i-\bar{x})^2}{n}\right]^{\frac{n}{2}}\left[\sum_{j=1}^{m}\frac{(y_j-\bar{y})^2}{m}\right]^{\frac{m}{2}}}{\left[\sum_{i=1}^{n}\left(x_i-\frac{n\bar{x}+m\bar{y}}{n+m}\right)^2+\sum_{j=1}^{m}\left(y_j-\frac{n\bar{y}+m\bar{y}}{n+m}\right)^2\right]^{\frac{n+m}{2}}}$$

Let $u = \frac{n\bar{y}+m\bar{y}}{n+m}$. Then, the likelihood ratio for testing $H_0:\theta_1=\theta_2$ and $\theta_3=\theta_4$ against the alternatives is given by

$$\frac{\left[\sum_{i=1}^{n}\frac{(x_i-\bar{x})^2}{n}\right]^{\frac{n}{2}}\left[\sum_{j=1}^{m}\frac{(y_j-\bar{y})^2}{m}\right]^{\frac{m}{2}}}{\left[\frac{\sum_{i=1}^{n}(x_i-u)^2+\sum_{j=1}^{m}(y_j-u)^2}{n+m}\right]^{\frac{n+m}{2}}}.$$

[b.] Show that the likelihood ratio test for testing $H_0:\theta_3=\theta_4$, where θ_1 and θ_2 are unspecified, against $H_1:\theta_3\neq\theta_4$ where θ_1 and θ_2 are unspecified can be based on the random variable

$$F = \frac{\frac{1}{n-1}\sum_{i=1}^{n}(x_i-\bar{x})^2}{\frac{1}{m-1}\sum_{i=1}^{m}(y_i-\bar{y})^2}.$$

The sample spaces are $W=\{(\theta_1,\theta_2,\theta_3,\theta_4),-\infty<\theta_1<\infty,-\infty<\theta_2<\infty,0<\theta_3=\theta_4<\infty\}$ and $\{(\theta_1,\theta_2,\theta_3,\theta_4),-\infty<\theta_1<\infty,-\infty<\theta_2<\infty,0<\theta_3<\infty,0<\theta_4<\infty\}$. Under W,

$$L(\underline{\theta}_W|\underline{x},\underline{y}) = \left(\frac{1}{2\pi}\right)^{\frac{n+m}{2}} \left(\frac{1}{\theta_3}\right)^{\frac{n+m}{2}} \exp\left\{-\frac{1}{2\theta_3}\left[\sum_{i=1}^{n}(x_i-\theta_1)^2 + \sum_{i=1}^{m}(y_i-\theta_2)^2\right]\right\}.$$

Consider,

$$\log L(\underline{\theta}_W|\underline{x},\underline{y}) = -\frac{n+m}{2}\log 2\pi\theta_3 - \frac{1}{2\theta_3}\left[\sum_{i=1}^{n}(x_i-\theta_1)^2 + \sum_{i=1}^{m}(y_i-\theta_2)^2\right]$$

$$\frac{d}{d\theta_1}\log L(\underline{\theta}_W|\underline{x},\underline{y}) = -\frac{1}{2\theta_3}(2)\sum_{i=1}^{n}(x_i-\theta_1)(-1) = 0 \Rightarrow \theta_1 = \bar{x}.$$

$$\frac{d}{d\theta_2}\log L(\underline{\theta}_W|\underline{x},\underline{y}) = -\frac{1}{2\theta_3}(2)\sum_{i=1}^{m}(y_i-\theta_2)(-1) = 0 \Rightarrow \theta_2 = \bar{y}.$$

$$\frac{d}{d\theta_3}\log L(\underline{\theta}_W|\underline{x},\underline{y}) = -\frac{n+m}{2}\frac{1}{2\pi\theta_3}2\pi + \frac{1}{2\theta_3^2}\left[\sum_{i=1}^{n}(x_i-\theta_1)^2 + \sum_{i=1}^{m}(y_i-\theta_2)^2\right] \Rightarrow$$

$$\theta_3 = \frac{\sum_{i=1}^{n}(x_i-\theta_1)^2 + \sum_{i=1}^{m}(y_i-\theta_2)^2}{n+m}.$$

Consider

$$\lambda = \frac{L(\underline{\theta}_W|\underline{x},\underline{y})}{L(\underline{\theta}_\Omega|\underline{x},\underline{y})} = \frac{(n+m)^{\frac{n+m}{2}}}{n^{n/2}m^{m/2}} \frac{\left(\frac{1}{n}\sum_{i=1}^{n}(x_i-\bar{x})^2\right)^{\frac{n}{2}} \left(\frac{1}{m}\sum_{i=1}^{m}(y_i-\bar{y})^2\right)^{\frac{m}{2}}}{\left(\sum_{i=1}^{n}(x_i-\bar{x})^2 + \sum_{i=1}^{m}(y_i-\bar{y})^2\right)^{\frac{n+m}{2}}} =$$

$$\frac{(n+m)^{\frac{n+m}{2}}}{n^{n/2}m^{m/2}} \frac{1}{\left(\frac{\sum_{i=1}^{n}(x_i-\bar{x})^2+\sum_{i=1}^{m}(y_i-\bar{y})^2}{\frac{1}{n}\sum_{i=1}^{n}(x_i-\bar{x})^2}\right)^{\frac{n}{2}} \left(\frac{\sum_{i=1}^{n}(x_i-\bar{x})^2+\sum_{i=1}^{m}(y_i-\bar{y})^2}{\frac{1}{m}\sum_{i=1}^{m}(y_i-\bar{y})^2}\right)^{\frac{m}{2}}} =$$

$$\frac{(n+m)^{\frac{n+m}{2}}}{n^{n/2}m^{m/2}} \frac{1}{\left[n\left(1+\frac{\sum_{i=1}^{m}(y_i-\bar{y})^2}{\sum_{i=1}^{n}(x_i-\bar{x})^2}\right)\right]^{\frac{n}{2}} \left[m\left(1+\frac{\sum_{i=1}^{n}(x_i-\bar{x})^2}{\sum_{i=1}^{m}(y_i-\bar{y})^2}\right)\right]^{\frac{m}{2}}} =$$

$$\frac{(n+m)^{\frac{n+m}{2}}}{n^{n/2}m^{m/2}} \frac{1}{\left[n\left(1+\frac{1}{\frac{\sum_{i=1}^{n}(x_i-\bar{x})^2}{\sum_{i=1}^{m}(y_i-\bar{y})^2}}\right)\right]^{\frac{n}{2}} \left[m\left(1+\frac{\sum_{i=1}^{n}(x_i-\bar{x})^2}{\sum_{i=1}^{m}(y_i-\bar{y})^2}\right)\right]^{\frac{m}{2}}} =$$

$$\frac{(n+m)^{\frac{n+m}{2}}}{n^{n/2}m^{m/2}} \frac{1}{\left[n\left(1+\frac{1}{\left(\frac{n-1}{m-1}\right)\frac{\sum_{i=1}^{n}(x_i-\bar{x})^2 \Big/ (n-1)}{\sum_{i=1}^{m}(y_i-\bar{y})^2 \Big/ (m-1)}}\right)\right]^{\frac{n}{2}} \left[m\left(1+\left(\frac{n-1}{m-1}\right)\frac{\sum_{i=1}^{n}(x_i-\bar{x})^2 \Big/ (n-1)}{\sum_{i=1}^{m}(y_i-\bar{y})^2 \Big/ (m-1)}\right)\right]^{\frac{m}{2}}}.$$

Therefore,

$$\lambda = \frac{(n+m)^{\frac{n+m}{2}}}{n^{n/2}m^{m/2}} \frac{1}{\left[n\left(1+\frac{m-1}{(n-1)F}\right)\right]^{\frac{n}{2}} \left[m\left(1+\frac{(m-1)F}{(n-1)}\right)\right]^{\frac{m}{2}}}$$

c. If $\theta_3 = \theta_4$ argue that the F statistic in part (b) is independent of the T statistic of Example 2 in this section of the text book.

$$F = \frac{\frac{1}{n-1}\sum_{i=1}^{n}(x_i-\bar{x})^2}{\frac{1}{m-1}\sum_{i=1}^{m}(y_i-\bar{y})^2} \sim F(n-1, m-1)$$

and from Example 2

$$T = \frac{\sqrt{\frac{nm}{n+m}}(\bar{x}-\bar{y})}{\sqrt{\frac{\sum_{i=1}^{n}(x_i-\bar{x})^2+\sum_{i=1}^{m}(y_i-\bar{y})^2}{n+m-2}}} \sim t(n+m-2).$$

From Chapter 4 in the text book, we consider the moment generating functions of $\bar{x}, x_1-\bar{x}, x_2-\bar{x}, ..., x_n-\bar{x}$ and we find that $M(t_0, t_1, t_2, ..., t_n) = M(t_0, 0, 0, ..., 0)M(0, t_1, t_2, ..., t_n)$. Therefore, $\bar{x}$ is independent of $(x_1-\bar{x}, x_2-\bar{x}, ..., x_n-\bar{x})$ Therefore, $\bar{x}$ is independent of $\frac{1}{n-1}\sum(x_i-\bar{x})^2$ and $\bar{y}$ is independent of $\frac{1}{m-1}\sum(y_i-\bar{y})^2$ Therefore $(\bar{x}-\bar{y})$ is independent of F and T is independent of F because F is a function of $\frac{1}{n-1}\sum(x_i-\bar{x})^2$ and $\frac{1}{m-1}\sum(y_i-\bar{y})^2$ and T is a function of $\bar{x}$ and $\bar{y}$. The prof said this proof is not complete.

9.37 Let $x \sim N(0, \theta)$ and in the notation of this section, let $\theta' = 4, \theta'' = 9, \alpha = 0.05$ and $\beta = 0.10$. Show that the sequential probability ratio test can be based upon the statistic $\sum x_1^2$. Determine $r_0(n)$ and $r_1(n)$. The pdf of x is

$$f(x) = \frac{1}{\sqrt{2\pi\theta}}e^{-\frac{1}{2\theta}x^2}, -\infty < x < \infty.$$

Therefore the likelihood function of θ is

$$\prod_{i=1}^{n} f(x_i|\theta) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\theta}}e^{-\frac{1}{2\theta}x_i^2} = (2\pi\theta)^{-\frac{n}{2}}e^{-\frac{1}{2\theta}\sum_{i=1}^{n}x_i^2}.$$

Consider

$$\lambda_n = \frac{L(\theta', n)}{L(\theta'', n)} = \frac{(2\pi\theta')^{-\frac{n}{2}}}{2\pi\theta'')^{-\frac{n}{2}}} \frac{e^{-\frac{1}{2\theta'}\sum_{i=1}^n x_i^2}}{e^{-\frac{1}{2\theta''}\sum_{i=1}^n x_i^2}} =$$

$$\frac{\left(\frac{9}{4}\right)^{\frac{n}{2}}}{\left(\frac{9}{4}\right)^{\frac{n}{2}}} \frac{e^{-\frac{1}{2}\left(\frac{1}{9}-\frac{1}{4}\right)\sum_{i=1}^n x_i^2}}{e^{-\frac{1}{2}\left(\frac{5}{36}\right)\sum_{i=1}^n x_i^2}}.$$

We continue sampling if $k_0 < \lambda < k_1$

$$k_0 < \left(\frac{9}{4}\right)^{\frac{n}{2}} e^{-\frac{1}{2}\left(\frac{5}{36}\right)\sum_{i=1}^n x_i^2} < k_1, \;\; \log k_0 < \frac{n}{2}\log\frac{9}{4} - \frac{1}{2}\left(\frac{5}{36}\right)\sum_{i=1}^n x_i^2 < \log k_1 \Rightarrow$$

$$\frac{n}{2}\log\frac{9}{4} - \log k_0 > \frac{1}{2}\left(\frac{5}{36}\right)\sum_{i=1}^n x_i^2 > \frac{n}{2}\log\frac{9}{4} - \log k_1 \Rightarrow$$

$$r_1 = 1.44\left(n\log\frac{3}{2} - \log k_0\right) > \sum_{i=1}^n x_i^2 > 1.44\left(n\log\frac{3}{2} - \log k_1\right) = r_0.$$

We reject H_0 if $\lambda_n \le r_0$ or if $\lambda_n \ge r_1$. The sequential probability ratio test statistic is $\sum_{i=1}^n x_i^2$. Let $\alpha_a = 0.05, \beta_a = 0.10$ $r_0 = \frac{\alpha_a}{1-\beta_a}$ and $r_1 = \frac{1-\alpha_a}{\beta_a}$. Therefore, $k_0 = \frac{0.05}{1-0.10} = \frac{0.05}{0.9} = \frac{0.5}{9}$, $k_1 = \frac{1-0.05}{0.1} = 9.5$, $r_0(n) = 14.4[n\log(1.5) - \log(9.5)]$, $r_1(n) = 14.4[n\log(1.5) + \log(18)]$.

9.39 Let the independent random variables y and z be $N(\mu_1, 1)$ and $N(\mu_2, 1)$. Let $\theta = \mu_1 - \mu_2$. Let us observe independent observations from each distribution, say $y_1, y_2, ..., y_n$ and $z_1, z_2, ..., z_n$. To test sequentially the hypothesis $H_0 : \theta = 0$ against $H_1 : \theta = \frac{1}{2}$ use the sequence $x_i = y_i - z_i, i = 1, 2, ..., n$. If $\alpha_a = \beta_a = 0.05$, show that the test can be based upon $\bar{x} = \bar{y} - \bar{z}$. Find $r_0(n)$ and $r_1(n)$. Solution: We know that $x_i = y_i - z_i \sim N(\theta, 2)$. The pdf of x is

$$f(x) = \frac{1}{\sqrt{2\pi}\sqrt{2}} e^{-\frac{1}{2}\frac{(x-\theta)^2}{2}} = \frac{1}{\sqrt{4\pi}} e^{-\frac{1}{4}(x-\theta)^2}.$$

Therefore, a likelihood function of θ is

$$L(\theta|n) = \prod_{i=1}^n f(x_i, \theta) = \prod_{i=1}^n (4\pi)^{-\frac{1}{2}} e^{-\frac{1}{4}(x_i-\theta)^2} = (4\pi)^{-\frac{n}{2}} e^{-\frac{1}{4}\sum_{i=1}^n (x_i-\theta)^2}.$$

Consider $H_0 : \theta = 0$ against $H_1 : \theta = \frac{1}{2}$. Consider

$$\lambda_n = \frac{L(\theta', n)}{L(\theta'', n)} = \frac{e^{-\frac{1}{4}\sum x_i^2}}{e^{-\frac{1}{4}\sum\left(x_i-\frac{1}{2}\right)^2}} = \frac{e^{-\frac{1}{4}\sum x_i^2}}{e^{-\frac{1}{4}\sum x_i^2 + \frac{1}{4}\sum x_i - \frac{n}{16}}} = e^{\frac{n}{16} - \frac{n\bar{x}}{4}}.$$

We continue sampling if $k_0 < \lambda_n < k_1$ or $k_0 < e^{\frac{n}{16} - \frac{n\bar{x}}{4}} < k_1 \Rightarrow \log k_0 < \frac{n}{16} - \frac{n\bar{x}}{4} < \log k_1 \Rightarrow \log k_0 - \frac{n}{16} < -\frac{n\bar{x}}{4} < \log k_1 - \frac{n}{16} \Rightarrow -\frac{4}{n}\left(\log k_0 - \frac{n}{16}\right) > \bar{x} > -\frac{4}{n}\left(\log k_1 - \frac{n}{16}\right) \Rightarrow r_1(n) = \frac{1}{4} - \frac{4}{n}\log k_0 > \bar{x} > \frac{1}{4} - \frac{4}{n}\log k_1 = r_0(n)$. We reject H_0 if $\lambda_n \le k_0 \Rightarrow \bar{x} \ge \frac{1}{4} - \frac{4}{n}\log k_0$. We accept H_0 if $\lambda_n \ge k_1 \Rightarrow \bar{x} \le \frac{1}{4} - \frac{4}{n}\log k_1$. This test can be based on $\bar{x} = \bar{y} - \bar{z}$. Let $\alpha_n = 0.05$ and $\beta_n = 0.05$. $k_0 = \frac{\alpha_n}{1-\beta_n} = \frac{0.05}{1-0.05} = \frac{5}{95} = \frac{1}{19}$, $k_1 = \frac{1-\alpha_n}{\beta_n} = \frac{0.95}{0.05} = 19$. Therefore $r_0 = \frac{1}{4} - \frac{4}{n}\log k_0 = \frac{1}{4} - \frac{4}{n}\log\frac{1}{19} = \frac{1}{4} + \frac{4}{n}\log 19$. $r_1(n) = \frac{1}{4} - \frac{4}{n}\log k_1 = \frac{1}{4} - \frac{4}{n}\log 19$.

14.30 2-Way ANOVA (Con't)

Our estimators are $\widehat{\alpha}_i = \bar{x}_{i\cdot\cdot} - \bar{x}$ and $\widehat{\beta}_j = \bar{x}_{\cdot j\cdot} - \bar{x}$, etc. The model statement is $x_{ijk} = \mu_{ij} + e_{ijk} = \mu + \alpha_i + \beta_j + \delta_{ij} + e_{ijk}$. $\theta' = (\mu_1\alpha_1, ..., \alpha_a, ..., \delta_{ab})$. $S = \sum(x_{ijk} - \mu_{ij})^2 = \sum(x_{ijk} - \bar{x}_{ij\cdot})^2 + abc(\mu - \bar{x})^2 + bc(\alpha_i - \widehat{\alpha}_i)^2 + ac\sum(\beta_j - \widehat{\beta}_j)^2 + c\sum(\delta_{ij} - \widehat{\delta}_{ij})^2$. Under $\Omega : \alpha_i = \widehat{\alpha}_i, \beta_j = \widehat{\beta}_j, \delta_{ij} = \widehat{\delta}_{ij}$, and $\mu = \bar{x}$ minimizes S. Under $H_A : \alpha_i = 0, \forall i$, all $\widehat{\beta}_j$, and $\widehat{\delta}_{ij}$ stay the same. So, $S_\Omega = \sum(x_{ijk} - \bar{x}_{ij\cdot})^2 = S(\widehat{\theta}_\Omega)$. $S_A = \sum(x_{ijk} - \bar{x}_{ij\cdot})^2 + bc\sum\widehat{\alpha}_i^2$. $S_B = \sum(x_{ijk} - \bar{x}_{ij\cdot})^2 + ac\sum\widehat{\beta}_j^2$. $S_{AB} = \sum(x_{ijk} - \bar{x}_{ij\cdot})^2 + c\sum_{i,j}\widehat{\delta}_{ij}^2$. $\lambda = \left(\frac{\widehat{\sigma}_\Omega^2}{\widehat{\sigma}_W^2}\right)^{\frac{n}{2}}$, where $\widehat{\sigma}_\Omega^2 = \frac{S_\Omega}{n}$ $\Omega \in A, B, AB$, $\widehat{\sigma}_A^2 = \frac{S_A}{n}$, and so on. $\lambda = \left(\frac{S_\Omega}{S_A}\right)^{\frac{n}{2}} = \left(\frac{S_\Omega}{S_\Omega + bc\sum\widehat{\alpha}_i^2}\right)^{\frac{n}{2}} = \frac{1}{1+\frac{bc\sum\widehat{\alpha}_i^2}{S_\Omega}}$. $\lambda \le \lambda_0 \Rightarrow \frac{bc\sum\widehat{\alpha}_i^2}{S_\Omega} \ge k \Rightarrow \frac{bc\sum\widehat{\alpha}_i^2}{S_\Omega} = \frac{bc\sum(\bar{x}_{i\cdot\cdot}-\bar{x})^2}{\sum(x_{ijk}-\bar{x}_{ij\cdot})^2}$. Note that $\bar{e}_{i\cdot\cdot} \sim N\left(0, \frac{\sigma^2}{bc}\right)$ and $\bar{e}_{i\cdot\cdot}$ are iid. $\sum(x_{ijk} - \bar{x}_{ij\cdot})^2$ is independent of $\bar{x}_{ij\cdot}, i = 1, ..., a; j = 1, ..., b$. $\sum(\bar{x}_{i\cdot\cdot} - \bar{x})^2$ is a function of $\{\bar{x}_{ij\cdot}\}$. We know that for fixed (i, j), $\sum_k \frac{(x_{ijk}-\bar{x}_{ij\cdot})^2}{\sigma^2} \sim \chi^2(c-1)$ and $\frac{S_\Omega}{\sigma^2}\sum_{i,j,k}\frac{(x_{ijk}-\bar{x}_{ij\cdot})^2}{\sigma^2} \sim \chi^2[ab(c-1)]$. Getting back to the model, the alternative hypothesis is $H_A : \alpha_i = 0$. $\bar{x}_{i\cdot\cdot} = \mu + \alpha_i + \bar{e}_{i\cdot\cdot}$. $\bar{x} = \mu + \bar{e}$. $\sum(\bar{x}_{i\cdot\cdot} - \bar{x})^2 = \sum\alpha_i^2 + \sum(\bar{e}_{i\cdot\cdot} - \bar{e})^2 + 2\sum\alpha_i(\bar{e}_{i\cdot\cdot} - \bar{e})$. If H_A is true, then $bc\sum\frac{(x_{i\cdot\cdot}-\bar{x})^2}{\sigma^2} = bc\sum\frac{(\bar{e}_{i\cdot\cdot}-\bar{e})^2}{\sigma^2} \sim \chi^2(a-1)$.

$$\frac{\frac{bc\sum(\bar{x}_{i\cdot\cdot}-\bar{x})^2}{a-1}}{\frac{\sum(x_{ijk}-\bar{x}_{ij\cdot})^2}{ab(c-1)}} = F \sim F[a-1, ab(c-1)].$$

We reject for large values of F. The ANOVA table follows.

Source	D.F.	S.S.	M(SS)	E(MSS)	F
Levels of A	$a-1$	Q_2	$\frac{Q_2}{a-1}$	$\sigma^2 + \frac{bc}{a-1}\sum\alpha_i^2$	$\frac{Q_2/(a-1)}{Q_6/[ab(c-1)]}$
Levels of B	$b-1$	Q_4	$\frac{Q_4}{b-1}$	$\sigma^2 + \frac{ac}{b-1}\sum\beta_j^2$	$\frac{Q_4/(b-1)}{Q_6/[ab(c-1)]}$
Interaction	$(a-1)(b-1)$	Q_5	$\frac{Q_5}{(a-1)(b-1)}$	$\sigma^2 + \frac{c}{(a-1)(b-1)}\sum\delta_{ij}^2$	$\frac{Q_5/[(a-1)(b-1)]}{Q_6/[ab(c-1)]}$
Error	$ab(c-1)$	Q_6	$\frac{Q_6}{ab(c-1)}$	σ^2	
Total	abc-1	Q			

$Q = \sum(x_{ijk} - \bar{x})^2 = bc\sum(\bar{x}_{i\cdot\cdot} - \bar{x})_A^2 + ac\sum(\bar{x}_{\cdot j\cdot} - \bar{x})_B^2 + c\sum(\bar{x}_{ij\cdot} - \bar{x}_{i\cdot\cdot} - \bar{x}_{\cdot j\cdot} + \bar{x})_{AB}^2 + \overbrace{\sum(x_{ijk} - \bar{x}_{ij\cdot})^2}^{\text{pure var.}} = Q_2 + Q_4 + Q_5 + Q_6$. $E\left[\frac{\sum(e_{i\cdot\cdot}-\bar{e})^2}{a-1}\right] = \frac{\sigma^2}{bc}$. To find $E[MSS] : E[bc\sum(x_{i\cdot\cdot} - \bar{x})^2] = bc\sum\alpha_i^2 + \frac{bc\sigma^2(a-1)}{bc} + 0$. Divide by $a-1$ to get $\frac{bc}{a-1}\sum\alpha_1^2 + \sigma^2$. We should be able to find the distributions and expected values of the above ANOVA table. The interaction Q_5 is the most difficult, and it must be deduced that it has a χ^2 distribution.

14.31 Two-Way ANOVA with $c = 1$

The model statement is $x_{ij} = \mu + \alpha_i + \beta_j + \gamma_{ij} + e_{ij}$. The number of parameters is $ab + 1$. The number of observations is ab. We must assume something. Assume that $\gamma_{ij} = 0$ (no interaction term). Then the model statement is $x_{ij} = \mu + \alpha_i + \beta_j + e_{ij}$. We have $1 + (a-1) + (b-1) + 1 = a + b$ parameters. $Q = \sum(x_{ij} - \bar{x})^2 = b\sum\widehat{\alpha}_i^2 + a\sum\widehat{\beta}_j^2 + \sum(x_{ij} - \bar{x}_{i\cdot} - \bar{x}_{\cdot j} + \bar{x})^2 \Rightarrow Q = Q_2 + Q_4 + Q_5$. The ANOVA table follows.

Source	DF	SS	F	$E(MS)$
A	$a-1$	Q_2	$\frac{Q_2/(a-1)}{Q_5/(a-1)(b-1)}$	$\sigma^2 + \frac{b}{a-1}\sum \alpha_i^2$
B	$b-1$	Q_4		
Error	$(a-1)(b-1)$	Q_5		σ^2
Total	$ab-1$	Q		

$\sum(x_{ij} - \bar{x}_{i\cdot} - \bar{x}_{\cdot j} + \bar{x})^2 = \sum(e_{ij} - \bar{e}_{i\cdot} - \bar{e}_{\cdot j} + \bar{x})^2 \sim \chi^2$ is always true.

14.32 Regression Problem

We are interested in the best predictor of y for a given x. So, minimizing $E[y-h(x)]^2$, where $h(x)$ is the predictor of y. $E(y) = \mu_y$. If $E(y|x) = h(x)$ then, it is minimized. Proof: $E[y-h(x)]^2 = E[y - E(y|x) + E(y|x) - h(x)]^2 = E[y - E(y|x)]^2 + E[E(y|x) - h(x)]^2 + 0$. If $\begin{pmatrix} y \\ x \end{pmatrix}$ has a *bivariate normal distribution,* then $E(y|x) = \alpha^* + \beta x = \alpha + \beta(x - \bar{x})$. The model $y = \alpha + \beta(x-\bar{x}) + e$ is the linear model and $E(e) = 0$, $Var(e) = Var(y) = \sigma^2$. $(y_1, x_1), (y_2, x_2), ..., (y_n.x_n)$ is a random sample. $\bar{x} = \sum \frac{x_i}{n}$. Then, we minimize $\sum_{i=1}^n [y_i - \alpha - \beta(x_i - \bar{x})]^2$ to get the *least squares estimator* of α and β. If $y|x \sim N[\alpha + \beta(x-\bar{x}), \sigma^2]$ then the mle is the same as the least squares estimators. $\widehat{\alpha} = \bar{y}$, $\widehat{\beta} = \frac{y_i(x_i - \bar{x})}{\theta^2}$, $\theta^2 = \sum_{i=1}^n (x_i - \bar{x})^2$. Assuming normality, then $e_1, e_2, ..., e_n$ are iid $N(0, \sigma^2)$. $E(\widehat{\alpha}) = E(\bar{y}) = E[\alpha + \bar{e}] = \alpha$. $Var(\widehat{\alpha}) = Var(\bar{y}) = \frac{\sigma^2}{n}$. $E(\widehat{\beta}) = \frac{\sum(x_i - \bar{x})}{\theta^2} E(y_i) = \frac{\sum(x_i-\bar{x})}{\theta^2}[\alpha + \beta(x_i - \bar{x})] = \frac{\beta}{\theta^2}\sum(x_i - \bar{x})^2 = \beta$. $Var(\widehat{\beta}) = \frac{\sum(x_i-\bar{x})^2}{\theta^2} Var(y_i) = \sigma^2 \frac{\theta^2}{\theta^4} = \frac{\sigma^2}{\theta^2}$. $\widehat{\beta} \sim N\left(\beta, \frac{\sigma^2}{\theta^2}\right)$. The mle of σ^2 is $\widehat{\sigma}^2 = \frac{1}{n}\sum(y_i - \widehat{y}_i)^2$, $\widehat{y}_i = \widehat{\alpha} + \widehat{\beta}(x_i - \bar{x})$ and it is unbiased. The unbiased estimator is $\widetilde{\sigma}^2 = \frac{1}{n-2}\sum(y_i - \widehat{y}_i)^2$. By adding and subtracting $\widehat{y}_i$ then, $\sum e_i^2 = \sum[y_i - \alpha - \beta(x_i - \bar{x})]^2 = \sum(y_i - \widehat{y}_i)^2 + (\widehat{\beta} - \beta)^2 \sum(x_i - \bar{x})^2 + n(\bar{y} - \alpha)^2$. We know that $\frac{\sum e_i^2}{\sigma^2} \sim \chi^2(n)$ and that $\frac{(\widehat{\beta}-\beta)^2\theta^2}{\sigma^2} \sim \chi^2(1)$ and that $\frac{n(\bar{y}-\alpha)^2}{\sigma^2} \sim \chi^2(1) \Rightarrow \sum \frac{(y_i - \widehat{y}_i)^2}{\sigma^2} \sim \chi^2(n-2)$ and it is independent of $\widehat{\beta} \Rightarrow E(\widetilde{\sigma}^2) = \sigma^2$.

To test the hypothesis $H_0 : \beta = 0$, the test statistic is $t = \frac{(\widehat{\beta}-0)}{\widetilde{\sigma}}\theta^2 \sim t(n-2)$ for one and two sided tests. For two sided tests only, $t^2 \sim F(1, n-2)$. For a given $x = x_0$, estimate y_0. We know that $E(y_0|x_0) = \alpha + \beta(x_0 - \bar{x})$. The estimate for $E(y_0|x_0)$ is given by $\widehat{\alpha} + \widehat{\beta}(x_0 - \bar{x})$. Then, $\widehat{y}_0 = \widehat{\alpha} + \widehat{\beta}(x_0 - \bar{x})$. $E(\widehat{y}_0) = E(\widehat{\alpha}) + E(\widehat{\beta})(x_0 - \bar{x}) = \alpha + \beta(x_0 - \bar{x}) = E(y_0)$. y_0 is a random variable. Given $x_1, x_2, ..., x_n$, and x_0, if $E(\widehat{y}_0 - y_0) = E(\widehat{y}_0) - E(y_0) = 0$, then $\widehat{y}_0$ is an unbiased estimator for y_0. $E(y|x) = \alpha + \beta(x - \bar{x})$. $E_{\bar{x}}[\alpha + \beta(x - \bar{x})] = \alpha + \beta(x - \mu_x)$ and $E(y|x) = \mu_y + \beta(x - \bar{x})$.

To find the confidence intervals, $Var(\widehat{y}_0) = Var[\widehat{\alpha} + \widehat{\beta}(x_0 - \bar{x})] = Var(\widehat{\alpha}) + (x_0 - \bar{x})^2 Var(\widehat{\beta})$ because $\widehat{\alpha}$ and $\widehat{\beta}$ are independent. $Var(\widehat{y}_0) = \frac{\sigma^2}{n} + (x_0 - \bar{x})^2 \frac{\sigma^2}{\theta^2} = \frac{\sigma^2}{n}\left[1 + \frac{(x_0-\bar{x})^2}{s_x^2}\right]$, where $s_x^2 = \frac{1}{n}\sum_{i=1}^n (x_i - \bar{x})^2$. Note that as s_x^2 increases, then $Var(\widehat{y}_0)$ decreases. Therefore, use $\frac{n}{2}$ observations at a and $\frac{n}{2}$ observations at b. The confidence interval of $\alpha + \beta(x_0 - \bar{x}) = E(y_0|x_0)$ is

$$\frac{y_0 - [E(y_0|x_0)]}{\left[\frac{\widetilde{\sigma}^2}{n}\left(1 + \frac{(x_0-\bar{x})^2}{s_x^2}\right)\right]^{\frac{1}{2}}} \sim t(n-2).$$

Therefore, the confidence interval is $(1-\alpha)100\%$ of $E(y_0|x_0)$

$$\widehat{y}_o \pm t_{\alpha/2}(n-2)\widetilde{\sigma}\left[\frac{1}{n}\left(1 + \frac{(x_0 - \bar{x})^2}{s_x^2}\right)\right]^{\frac{1}{2}}$$

For any new y_0, $E(\widehat{y}_0 - y_0) = 0$ and $Var(\widehat{y}_0 - y_0) = Var(\widehat{y}_0) - Var(y_0) = \sigma^2\left[1 + \frac{1}{n} + \frac{(x_0-\bar{x})^2}{\theta^2}\right] = \frac{\sigma^2}{n}\left[n + 1 + \frac{(x_0-\bar{x})^2}{s_x^2}\right]$.

$$\frac{\widehat{y}_o - y_0}{\widetilde{\sigma}\left[1+\frac{1}{n}+\frac{(x_0-\bar{x})^2}{\theta^2}\right]^{\frac{1}{2}}} \sim t(n-2).$$

Thus, the confidence interval for y_0 is

$$\widehat{y}_0 \pm t_{\alpha/2}(n-2)\widetilde{\sigma}\left[1+\frac{1}{n}+\frac{(x_0-\bar{x})^2}{\theta^2}\right]^{\frac{1}{2}}$$

which is a wider interval.

The relationship between ρ (the correlation coefficient) of (x,y) $\rho = \frac{Cov(x,y)}{\sigma_x\sigma_y}$, $Cov(x,y) = E[(x-\mu_x)(y-\mu_y)] = E[xy]-\mu_x\mu_y$, $\sigma_x^2 = Var(x)$. Suppose that we have the sample $(x_1,y_1),...,(x_n,y_n)$ and it is a bivariate random sample. Then, the sample correlation coefficient r is $r = \frac{s_{xy}}{s_x s_y}$ where $s_{xy} = \frac{1}{n}\sum_{i=1}^n(x_i-\bar{x})(y_i-\bar{y})$ and $s_x^2 = \frac{1}{n}\sum_{i=1}^n(x_i-\bar{x})^2$. Consider the model $y = \alpha^* + \beta x + e$. $\sigma_{xy} = Cov(x,y) = E[y(x-\mu_x)] = E_x[(x-\mu_x)E(y|x)] = E_x[(x-\mu_x)(\alpha^*+\beta x)] = \alpha^* E(x-\mu_x) + \beta E[x(x-\mu_x)] = 0 + \beta\sigma_x^2$. $Var(x) = E[x-\mu_x]^2 = E(x-\mu_x)(x-\mu_x)] = E[x(x-\mu_x)]$. So, $\frac{\sigma_{xy}}{\sigma_x^2} = \beta$. Then, $\rho = \frac{\sigma_{xy}}{\sigma_x\sigma_y} = \frac{\sigma_{xy}}{\sigma_x^2}\frac{\sigma_x}{\sigma_y} = \beta\frac{\sigma_x}{\sigma_y}$. So, if $\rho = 0 \Leftrightarrow \beta = 0$.

14.33 Homework and Answers

10.3 Let $x_1, x_2, ..., x_n$ be a random sample from a normal distribution $N(\mu,\sigma^2)$. Show that

$$\sum_{i=1}^n(x_i-\bar{x})^2 = \sum_{i=2}^n(x_i-\bar{x}')^2 + \frac{(n-1)}{n}(x_1-\bar{x}')^2$$

where $\bar{x} = \sum_{i=1}^n \frac{x_i}{n}$ and $\bar{x}' = \sum_{i=2}^n \frac{x_i}{n-1}$. HINT: Replace $x_i - \bar{x}$ by $(x_i-\bar{x}') - (x_1-\bar{x}')/n$. Show that $\sum_{i=2}^n(x_i-\bar{x}')^2/\sigma^2$ has a chi-square distribution with $n-2$ degrees of freedom. Prove that the two terms in the right-hand members are independent. What then is the distribution of $\frac{[(n-1)/n](x_1-\bar{x}')^2}{\sigma^2}$?

$$\sum_{i=1}^n(x_i-\bar{x})^2 = \sum_{i=1}^n\left[(x_i-\bar{x}') - \frac{(x_1-\bar{x}')}{n}\right]^2 =$$

$$\sum_{i=1}^n(x_i-\bar{x}')^2 - \frac{2\sum_{i=1}^n(x_i-\bar{x}')(x_1-\bar{x}')}{n} + \frac{\sum_{i=1}^n(x_1-\bar{x}')^2}{n^2} =$$

$$\sum_{i=1}^n(x_i-\bar{x}')^2 - 2\frac{(x_1-\bar{x}')}{n}\sum_{i=1}^n(x_i-\bar{x}') + \frac{n}{n^2}(x_1-\bar{x}')^2 =$$

$$\sum_{i=2}^n(x_i-\bar{x}')^2 + (x_1-\bar{x}')^2 - \frac{2(x_1-\bar{x}')}{n}\left[(x_1-\bar{x}') + \sum_{i=2}^n(x_i-\bar{x}')\right] =$$

$$\sum_{i=2}^n(x_i-\bar{x}')^2 + \frac{1}{n}(x_1-\bar{x}')^2 + \left[(x_1-\bar{x}')^2 - \frac{2}{n}(x_1-\bar{x}')^2 + \frac{1}{n}(x_1-\bar{x}')^2\right] =$$

$$\sum_{i=2}^{n}(x_i-\bar{x}')^2+\overbrace{(x_1-\bar{x}')^2-2(x_1-\bar{x}')\sum_{i=2}^{n}(x_i-\bar{x}')}^{\text{must be zero for proof to work}}+(x_1-\bar{x}')^2\left[1-\frac{1}{n}\right]-\frac{2(x_1-\bar{x}')}{n}\overbrace{\left[\sum_{i=2}^{n}x_i-(n-1)\bar{x}'\right]}^{=0}.$$

Therefore, $\sum_{i=1}^{n}(x_i-\bar{x})^2=\sum_{i=2}^{n}(x_i-\bar{x}')^2+\frac{(n-1)}{n}(x_1-\bar{x}')^2$. These are the quadratic form $x_i\sim N(\mu,\sigma^2)$ and from an example in Chapter 10 in the text book, we know that $\sum_{i=1}^{n}(x_i-\bar{x})^2/\sigma^2\sim\chi^2(n-1)$. Consider $x_1\sim N(\mu,\sigma^2)$ and $\bar{x}'=\frac{\sum_{i=2}^{n}x_i}{n-1}$. $E(\bar{x}')=\frac{1}{n-1}\sum_{i=2}^{n}E(x_i)=\frac{1}{n-1}(n-1)\mu=\mu$. $Var(\bar{x}')=\frac{1}{(n-1)^2}\sum_{i=2}^{n}Var(x_i)=\frac{1}{(n-1)^2}(n-1)\sigma^2=\frac{\sigma^2}{(n-1)}\Rightarrow\bar{x}'\sim N\left(\mu,\frac{\sigma^2}{n-1}\right)$. x_1 and $\bar{x}'$ are independent because $x_1,x_2,...,x_n$ are independent. The distribution of $\sum_{i=2}^{n}(x_i-\bar{x}')^2/\sigma^2$ is $\chi^2(n-2)$.

10.4 Let $x_{ijk}, i=1,2,...a; j=1,2,...,b; k=1,2,...,c$ be a random sample of size $n=abc$ from a normal distribution $N(\mu,\sigma^2)$. Let $\bar{x}=\sum_{k=1}^{c}\sum_{j=1}^{b}\sum_{i=1}^{a}x_{ijk}/n$ and $\bar{x}_{..}=\sum_{k=1}^{c}\sum_{j=1}^{b}x_{ijk}/(bc)$. Show that $\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{...})^2=\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{i..})^2+bc\sum_{i=1}^{c}(\bar{x}_{i..}-\bar{x}_{...})^2$. Show that $\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{i..})^2/\sigma^2$ has a chi-square distribution with $a(bc-1)$ degrees of freedom. Prove that the two terms in the right-hand member are independent. What, then, is the distribution of $bc\sum_{i=1}^{a}(\bar{x}_{i..}-\bar{x}_{...})^2/\sigma^2$?. Furthermore, let $\bar{x}_{.j.}=\sum_{k=1}^{c}\sum_{i=1}^{a}x_{ijk}/ac$ and $\bar{x}_{ij.}=\sum_{k=1}^{c}x_{ijk}/c$. Show that

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{...})^2=$$

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{ij.})^2+bc\sum_{i=1}^{a}(\bar{x}_{i..}-\bar{x}_{...})^2+ac\sum_{j=1}^{b}(\bar{x}_{.j.}-\bar{x}_{...})^2+c\sum_{i=1}^{a}\sum_{j=1}^{b}(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...})^2.$$

Show that the four terms in the right-hand term member, when divided by σ^2, are independent chi-square variables with $ab(c-1), a-1, b-1$, and $(a-1)(b-1)$ degrees of freedom respectfully.

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{...})^2=\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}\left[(x_{ijk}-\bar{x}_{i..})+(\bar{x}_{i..}-\bar{x}_{...})\right]^2=$$

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{i..})^2+2\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{i..})(\bar{x}_{i..}-\bar{x}_{...})+\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{i..}-\bar{x}_{...})^2.$$

Consider the cross product term

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{i..})(\bar{x}_{i..}-\bar{x}_{...})=$$

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}x_{ijk}\bar{x}_{i..}-\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}x_{ijk}\bar{x}_{...}-\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{i..})^2+\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}\bar{x}_{i..}\bar{x}_{...}=$$

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}x_{ijk}-\bar{x}_{...}\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}x_{ijk}-bc\sum_{i=1}^{a}(\bar{x}_{i..})^2+bc\bar{x}_{...}\sum_{i=1}^{a}\bar{x}_{i..}=$$

$$bc\sum_{i=1}^{a}\left(\bar{x}_{i..}\right)^2 - abc\left(\bar{x}_{...}\right)^2 - bc\sum_{i=1}^{a}\left(\bar{x}_{i..}\right)^2 + abc\left(\bar{x}_{...}\right)^2 = 0.$$

Therefore,

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{...})^2 = \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{i..})^2 + \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{i..}-\bar{x}_{...})^2 =$$

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{i..})^2 + bc\sum_{i=1}^{a}(\bar{x}_{i..}+\bar{x}_{...})^2.$$

Therefore, $x_{ijk} \sim N(\mu, \sigma^2), i = 1, ..., a; j = 1, ..., b; k = 1, ..., c; \sum_i\sum_j\sum_k(x_{ijk}-\bar{x}_{...})^2/\sigma^2 \sim \chi^2(abc-1)$ and $\bar{x}_{i..} \sim N\left(\mu, \frac{\sigma^2}{bc}\right) \Rightarrow bc\frac{\sum_{i=1}^{a}(\bar{x}_{i..}-\bar{x}_{...})^2}{\sigma^2} \sim \chi^2(a-1)$. Obviously, $\sum_i\sum_j\sum_k(x_{ijk}-\bar{x}_{i..})^2$ is non-negative. By using the theorem, we have $\sum_i\sum_j\sum_k(x_{ijk}-\bar{x}_{i..})^2 \sim \chi^2(r)$ where $r = (abc-1)-(a-1) = a(bc-1)$. Also, $\sum_i\sum_j\sum_k(x_{ijk}-\bar{x}_{i..})^2$ and $bc\sum_i(\bar{x}_{i..}-\bar{x}_{...})^2$ are independent.

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{...})^2 =$$

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}\left[(x_{ijk}-\bar{x}_{ij.}) + (\bar{x}_{i..}-\bar{x}_{...}) + (\bar{x}_{.j.}-\bar{x}_{...}) + (\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...})\right] =$$

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{ij.})^2 + \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{i..}-\bar{x}_{...})^2 + \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{.j.}-\bar{x}_{...}) +$$

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...})^2 + 2\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{ij.})(\bar{x}_{i..}-\bar{x}_{...}) +$$

$$2\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{ij.})(\bar{x}_{.j.}-\bar{x}_{...}) + 2\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{ij.})(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...}) +$$

$$2\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{i..}-\bar{x}_{...})(\bar{x}_{.j.}-\bar{x}_{...}) + 2\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{i..}-\bar{x}_{...})(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...}) +$$

$$2\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{.j.}-\bar{x}_{...})(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...}).$$

Consider the cross product terms

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{ij.})(\bar{x}_{i..}-\bar{x}_{...}) =$$

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}x_{ijk}\bar{x}_{i..}-\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}x_{ijk}\bar{x}_{...}-\sum_{i=1}^{a}\sum_{j=1}^{b}\overbrace{\sum_{k=1}^{c}\bar{x}_{ij.}}^{x_{ij.}}\bar{x}_{i..}+\sum_{i=1}^{a}\sum_{j=1}^{b}\overbrace{\sum_{k=1}^{c}\bar{x}_{ij.}}^{x_{ij.}}\bar{x}_{...}=$$

$$bc(\bar{x}_{i..})^2-abc(\bar{x}_{...})^2-bc(\bar{x}_{i..})^2+abc(\bar{x}_{...})^2=0.$$

Consider the cross product terms

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{ij.})(\bar{x}_{.j.}-\bar{x}_{...})=$$

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}x_{ijk}\bar{x}_{.j.}-\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}x_{ijk}\bar{x}_{...}-\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}\bar{x}_{ij.}\bar{x}_{.j.}+\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}\bar{x}_{ij.}\bar{x}_{...}=$$

$$ac(\bar{x}_{.j.})^2-abc(\bar{x}_{...})^2-ac(\bar{x}_{.j.})^2+abc(\bar{x}_{...})^2=0.$$

Consider the cross product terms

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{ij.})(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...})=\sum_{i=1}^{a}\sum_{j=1}^{b}(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...})\overbrace{\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{ij.})}^{=0}=0$$

Consider the cross product terms

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{i..}-\bar{x}_{...})(\bar{x}_{.j.}-\bar{x}_{...})=$$

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}\bar{x}_{i..}\bar{x}_{.j.}-\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}\bar{x}_{i..}\bar{x}_{...}-\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}\bar{x}_{...}\bar{x}_{.j.}+\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{...})^2=$$

$$c(x_{i..})x_{.j.}-bc(\bar{x}_{...})x_{i..}-ac\bar{x}_{...}x_{.j.}+abc(\bar{x}_{...})^2=ac(\bar{x}_{...})x_{.j.}-abc(\bar{x}_{...})^2-ac(\bar{x}_{...})x_{.j.}+abc(\bar{x}_{...})^2=0.$$

Consider the cross product terms

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{i..}-\bar{x}_{...})(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...})=\overbrace{\sum_{i=1}^{a}(\bar{x}_{i..}-\bar{x}_{...})}^{=0}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...})=0$$

Consider the cross product terms

$$\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{.j.}-\bar{x}_{...})(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...}) = \overbrace{\sum_{j=1}^{b}(\bar{x}_{.j.}-\bar{x}_{...})}^{=0}\sum_{i=1}^{a}\sum_{k=1}^{c}(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...}) = 0$$

So,

$$x_{ijk} \sim N(\mu,\sigma^2) \Rightarrow \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{...})^2/\sigma^2 \sim \chi^2(abc-1).$$

$$\bar{x}_{ij.} \sim N(\mu,\sigma^2) \Rightarrow \sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(x_{ijk}-\bar{x}_{ij.})^2/\sigma^2 \sim \chi^2[ab(c-1)].$$

$$\bar{x}_{i..} \sim N(\mu,\sigma^2/bc) \Rightarrow bc\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{i..}-\bar{x}_{...})^2/\sigma^2 \sim \chi^2(a-1).$$

$$\bar{x}_{.j.} \sim N(\mu,\sigma^2/ac) \Rightarrow ac\sum_{i=1}^{a}\sum_{j=1}^{b}\sum_{k=1}^{c}(\bar{x}_{.j.}-\bar{x}_{...})^2/\sigma^2 \sim \chi^2(b-1).$$

Obviously, $c\sum_i\sum_j\sum_k(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...})^2$ is non-negative by using the theorem. We have then $c\sum_i\sum_j\sum_k(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...})^2/\sigma^2 \sim \chi^2(r)$ where $r = (abc-1)-ab(c-1)-(a-1)-(b-1) = abc-1-abc+ab-a+1-b+1 = (a-1)(b-1)$. Also, $\sum_i\sum_j\sum_k(x_{ijk}-\bar{x}_{ij.})^2, bc\sum_{i=1}^{a}(\bar{x}_{i..}-\bar{x}_{...})^2, ac\sum_{j=1}^{b}(\bar{x}_{.j.}-\bar{x}_{...})^2$, and $c\sum_{i=1}^{a}\sum_{j=1}^{b}(\bar{x}_{ij.}-\bar{x}_{i..}-\bar{x}_{.j.}+\bar{x}_{...})^2$ are independent.

10.11 Let $y_i, i = 1,2,...,n$ denote independent random variables that are respectively, $\chi^2(r_i,\theta_i), i = 1,2,...,n$. Prove that $z = \sum_{i=1}^{n} y_i$ is $\chi^2\left(\sum_{i=1}^{n} r_i, \sum_{i=1}^{n}\theta_i\right)$. The mgf of y_i is $M_{y_i}(t) = e^{t\theta_i/(1-2t)}(1-2t)^{-\frac{r_i}{2}}$ where $t < \frac{1}{2}, \theta > 0$ and r_i are positive integers. Let $z = \sum_{i=1}^{n} y_i$. An mgf of Z is

$$M_z(t) = E(e^{tz}) = E(e^{t\sum_{i=1}^{n} y_i}) = \prod_{i=1}^{n} E(e^{ty_i}) = \prod_{i=1}^{n} M_{y_i}(t) = \prod_{i=1}^{n} e^{t\theta_i/(1-2t)}(1-2t)^{-\frac{r_i}{2}} =$$

$$\left[e^{\frac{t}{1-2t}\sum_{i=1}^{n}\theta_i}\right](1-2t)^{-\frac{\sum_{i=1}^{n} r_i}{2}} \Rightarrow \text{ is the mgf of a } \chi^2\left[\sum_{i=1}^{n} r_i, \sum_{i=1}^{n}\theta_i\right]$$

10.12 Compute the mean and the variance of a random variable that is $\chi^2(r,\theta)$. Let $x \sim \chi^2(r,\theta)$. An mgf of x is $M_x(t) = e^{t\theta/(1-2t)}(1-2t)^{-\frac{r}{2}}$ where $t < \frac{1}{2}$ and $\theta > 0$ and r is a positive number.

$$M_x'(t) = e^{t\theta/(1-2t)}\left(-\frac{r}{2}\right)(1-2t)^{-\frac{r}{2}-1}(-2) + (1-2t)^{-\frac{r}{2}}e^{t\theta/(1-2t)}\theta\left[\frac{(1-2t)(1)-t(-2)}{(1-2t)^2}\right] =$$

$$re^{t\theta(1-2t)}(1-2t)^{-\frac{r}{2}-1} + \theta e^{t\theta/(1-2t)}(1-2t)^{-\frac{r}{2}-2}.$$

Therefore, $E(x) = M_x'(0) = r+\theta$.

$$M_x''(t) = r\left[e^{t\theta/(1-2t)}\left(-\frac{r}{2}-1\right)(1-2t)^{-\frac{r}{2}-2}(-2) + (1-2t)^{-\frac{r}{2}-1}e^{t\theta/(1-2t)}\theta\left(\frac{1}{(1-2t)^2}\right)\right] +$$

$$\theta\left[e^{t\theta/(1-2t)}\left(-\frac{r}{2}-2\right)(1-2t)^{-\frac{r}{2}-3}(-2) + (1-2t)^{-\frac{r}{2}-2}e^{t\theta/(1-2t)}\theta\left(\frac{1}{(1-2t)^2}\right)\right] =$$

$$2r\left(\frac{r}{2}+1\right)e^{t\theta/(1-2t)}(1-2t)^{-\frac{r}{2}-2} + \theta r e^{t\theta/(1-2t)}(1-2t)^{-\frac{r}{2}-1} +$$

$$2\theta\left(\frac{r}{2}+2\right)e^{t\theta/(1-2t)}(1-2t)^{-\frac{r}{2}-3} + \theta^2 e^{t\theta/(1-2t)}(1-2t)^{-\frac{r}{2}-4}.$$

Therefore, $E(x^2) = M_x''(0) = 2r\left(\frac{r}{2}+1\right) + \theta r + 2\theta\left(\frac{r}{2}+2\right) + \theta^2$. Therefore, $Var(x) = E(x^2) - [E(x)]^2 = 2r\left(\frac{r}{2}+1\right) + \theta r + 2\theta\left(\frac{r}{2}+1\right) + \theta^2 - (r+\theta)^2 = r^2 + 2r + \theta r + r\theta + 4\theta + \theta^2 - r^2 - 2r\theta - \theta^2 = 2r + 4\theta$.

10.24 With the background of the two-way classification with $c > 1$ observations per cell, show that the maximum likelihood estimator of the parameters are $\widehat{\alpha}_i = \bar{x}_{i..} - \bar{x}_{...}, \widehat{\beta}_j = \bar{x}_{.j.} - \bar{x}_{...}, \widehat{\delta}_{ij} = \bar{x}_{ij.} - \bar{x}_{i..} - \bar{x}_{.j.} + \bar{x}_{...}$, and $\widehat{\mu} = \bar{x}_{...}$. Show that these are unbiased estimators of the respective parameters. Compute the variance of each estimator. We have $x_{ijk} = \mu + \alpha_i + \beta_j + \delta_{ij} + \epsilon_{ijk}, i = 1,...,a; j = 1,...,b; k = 1,...,c$ and $E(x_{ijk}) = \mu + \alpha_i + \beta_j + \delta_{ij}$. A likelihood function is $L = \left(\frac{1}{2\pi\sigma^2}\right)^{\frac{n}{2}} e^{-\frac{1}{2\sigma^2}\sum_i\sum_j\sum_k(x_{ijk}-\mu-\alpha_i-\beta_j-\delta_{ij})^2}$, $\log L = -\frac{n}{2}\log 2\pi\sigma^2 - \frac{1}{2\sigma^2}\sum_i\sum_j\sum_k(x_{ijk} - \mu - \alpha_i - \beta_j - \delta_{ij})^2$, $\frac{d}{d\mu}\log L = \frac{1}{\sigma^2}\sum_i\sum_j\sum_k(x_{ijk} - \mu - \alpha_i - \beta_j - \delta_{ij}) = 0$, $x_{...} - abc\mu - bc\sum_i\alpha_i - ac\sum_j\beta_j - c\sum_i\sum_j\delta_{ij} = 0 \Rightarrow \widehat{\mu} = \frac{x_{...}}{abc} = \bar{x}_{...}$. $E(\bar{x}_{...}) = \frac{1}{abc}\sum_i\sum_j\sum_k E(x_{ijk}) = \frac{1}{abc}\sum_i\sum_j\sum_k(\mu+\alpha_i+\beta_j+\delta_{ij}) = \frac{1}{abc}\left[abc\mu + bc\sum_i\alpha_i + ac\sum_j\beta_j + c\sum_i\sum_j\delta_{ij}\right] = \mu$. Therefore $\bar{x}_{...}$ is an unbiased estimator for μ. Consider the derivative $\frac{d}{d\alpha_i}\log L = \frac{1}{\sigma^2}\sum_j\sum_k(x_{ijk} - \mu - \alpha_i - \beta_j - \delta_{ij}) = 0$, $x_{i..} - bc\mu - bc\alpha_i - c\sum_j\beta_j - c\sum_j\delta_{ij} = 0$ $bc\alpha_i = x_{i..} - bc\mu \Rightarrow \alpha_i = \bar{x}_{i..} - \mu \Rightarrow \widehat{\alpha}_i = \bar{x}_{i..} - \bar{x}_{...}$ is the mle of α_i. $E(\bar{x}_{i..} - \bar{x}_{...}) = E(\bar{x}_{i..}) - E(\bar{x}_{...}) = \frac{1}{bc}\sum_j\sum_k E(x_{ijk}) - \mu = \frac{1}{bc}\sum_j\sum_k(\mu + \alpha_i + \beta_j + \delta_{ij}) - \mu = \frac{1}{bc}\left[bc\mu + bc\alpha_i + c\sum_j\beta_j + c\sum_j\delta_{ij}\right] - \mu = \mu + \alpha_i - \mu = \alpha_i \Rightarrow$ unbiased. Consider the derivative $\frac{d}{d\beta_j}\log L = \frac{1}{\sigma^2}\sum_i\sum_k(x_{ijk} - \mu - \alpha_i - \beta_j - \delta_{ij}) = 0$, $x_{.j.} - ac\mu - c\sum_i\alpha_i - ac\beta_j - c\sum_i\delta_{ij} = 0$ $\beta_j = \bar{x}_{.j.} - \mu \Rightarrow \widehat{\beta}_j = \bar{x}_{.j.} - \bar{x}_{...}$ is the mle of β_j. $E(\bar{x}_{.j.} - \bar{x}_{...}) = E(\bar{x}_{.j.}) - E(\bar{x}_{...}) = \frac{1}{ac}\sum_i\sum_k E(x_{ijk}) - \mu = \frac{1}{ac}\sum_i\sum_k(\mu + \alpha_i + \beta_j + \delta_{ij}) - \mu = \frac{1}{ac}\left[ac\mu + 0 + ac\beta_j + 0\right] - \mu = \mu + \beta_j - \mu = \beta_j \Rightarrow \widehat{\beta}_j = \bar{x}_{.j.} - \bar{x}_{...}$ is unbiased. Consider the derivative $\frac{d}{d\delta_{ij}}\log L = \frac{1}{\sigma^2}\sum_k(x_{ijk} - \mu - \alpha_i - \beta_j - \delta_{ij}) = 0$, $x_{.j.} - c\mu - c\alpha_i - c\beta_j - c\delta_{ij} = 0$ $\delta_{ij} = \bar{x}_{ij.} - \mu - \alpha_i - \beta_j \Rightarrow \widehat{\delta}_{ij} = \bar{x}_{ij.} - \bar{x}_{i..} - \bar{x}_{.j.} + \bar{x}_{...}$ is the mle. $E(\bar{x}_{ij.} - \bar{x}_{i..} - \bar{x}_{.j.} + \bar{x}_{...}) = E(\bar{x}_{ij.}) - E(\bar{x}_{i..}) - E(\bar{x}_{.j.}) + E(\bar{x}_{...}) = \frac{1}{c}\sum_{k=1}^{c}E(x_{ijk}) - (\mu + \alpha_i) - (\mu + \beta_j) + \mu = \frac{1}{c}\sum_{k=1}^{c}(\mu + \alpha_i + \beta_j + \delta_{ij}) - \alpha_i - \beta_j - \mu = \frac{1}{c}(c\mu + c\alpha_i + c\beta_j + c\delta_{ij}) - \alpha_i - \beta_j - \mu = \mu + \alpha_i + \beta_j + \delta_{ij} - \alpha_i - \beta_j - \mu = \delta_{ij} \Rightarrow \widehat{\delta}_{ij} = \bar{x}_{ij.} - \bar{x}_{i..} - \bar{x}_{.j.} + \bar{x}_{...}$ is unbiased. Therefore, $Var(\bar{x}_{...}) = \frac{1}{a^2b^2c^2}\sum_i\sum_j\sum_k Var(x_{ijk}) = \frac{abc\sigma^2}{a^2b^2c^2} = \frac{\sigma^2}{abc}$.

10.35 Let $Q = x_1x_2 - x_3x_4$ where x_1, x_2, x_3, and x_4 is a random sample of size four from a distribution which is $N(0, \sigma^2)$. Show that Q/σ^2 does not have a chi-square distribution. Find the mgf of Q/σ^2.

$$Q = x_1x_2 - x_3x_4 = (x_1\ \ x_2\ \ x_3\ \ x_4)\begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & 0 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}.$$

In this case,

$$A = \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & 0 \end{pmatrix}$$

and is symmetric. The rank of A is 2 which is less than $n = 4$. Does $A^2 = A$?

$$A^2 = AA = \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & 0 \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{pmatrix} \neq A.$$

By using Theorem 2 on page 484 of the text book, we know that Q/σ^2 does not have a chi-square distribution. From page 483 of the text book, we know that the mgf of $x'Ax/\sigma^2$ is given by

$$M(t) = |I - 2tA|^{-\frac{1}{2}}, |t| < h = \left| \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} - 2t \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & 0 \end{pmatrix} \right|^{-\frac{1}{2}} =$$

$$\begin{vmatrix} 1 & -t & 0 & 0 \\ -t & 1 & 0 & 0 \\ 0 & 0 & 1 & t \\ 0 & 0 & t & 1 \end{vmatrix}^{-\frac{1}{2}} = \left(1 \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & t \\ 0 & t & 1 \end{vmatrix} + t \begin{vmatrix} -t & 0 & 0 \\ 0 & 1 & t \\ 0 & t & 1 \end{vmatrix} \right)^{-\frac{1}{2}} = [(1 - t^2) + t(-t + t^3)]^{-\frac{1}{2}} =$$

$$(1 - t^2 - t^2 + t^4)^{-\frac{1}{2}} = (1 - 2t^2 + t^4)^{-\frac{1}{2}} = (1 - t^2)^{-1} = \frac{1}{(1-t)(1+t)}.$$

10.41 Let $\bar{x}$ and s^2 denote, respectively, the mean and the variance of a random sample of size n from a distribution which is $N(0, \sigma^2)$. a) If A denotes the symmetric matrix of $n\bar{x}^2$, show that $A = \frac{1}{n}P$, where P is the $n \times n$ matrix, each of whose elements is square to one. b) Demonstrate that A is idempotent and that the trace $tr(A) = 1$. Thus, $n\bar{x}^2/\sigma^2$ is $\chi^2(1)$. c) Show that the symmetric matrix B of ns^2 is $I - \frac{1}{n}P$. d) Demonstrate that B is idempotent and that $tr(B) = n - 1$. Thus, ns^2/σ^2 is $\chi^2(n-1)$, as previously proved. e) Show that the product matrix $A \times B$ is the zero matrix. To solve part a:

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i = \frac{1}{n}(1 \ 1 \ \cdots \ 1)_{1\times n} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}_{n\times 1} = \frac{1}{n}\underline{j}'x \text{ where } \underline{j}' = (1 \ 1 \ \cdots \ 1)_{1\times n}.$$

$$n\bar{x}^2 = n\left(\frac{1}{n}\underline{j}'x\right)\left(\frac{1}{n}\underline{j}'x\right) = x'\underline{j}\frac{1}{n}\underline{j}'x = x'\frac{1}{n}\underline{j}\,\underline{j}'x \Rightarrow A = \frac{1}{n}\underline{j}\,\underline{j}'.$$

Matrix A denotes the symmetric matrix of $n\bar{x}^2$, where P is

$$P = \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix}_{n\times n}$$

Consider

$$A = \frac{1}{n}\begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}(1\ 1\ 1\ \cdots\ 1) = \frac{1}{n}\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix}_{n\times n} = \frac{1}{n}P.$$

To solve part (b).

$$A^2 = AA = \frac{1}{n}\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix}\frac{1}{n}\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix} =$$

$$\frac{1}{n}\left(\frac{1}{n}\right)\begin{pmatrix} n & n & n & \cdots & n \\ n & n & n & \cdots & n \\ n & n & n & \cdots & n \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ n & n & n & \cdots & n \\ n & n & n & \cdots & n \end{pmatrix} = \frac{1}{n}\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix} = A.$$

Therefore matrix A is idempotent. Since A is idempotent, then $tr(A) = rank(A) = 1$. By using Theorem 2 on page 484 of the text book, we have $n\bar{x}^2/\sigma^2$ is $\chi^2(1)$ since A has a rank of 1. To solve part (c),

$$ns^2 = n\sum_{i=1}^{n}\frac{(x_i-\bar{x})^2}{n} = \sum_{i=1}^{n}x_i^2 - n\bar{x}^2 = (x_1\ \ x_2\ \ \cdots\ \ x_n)\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} - x'\frac{1}{n}Px =$$

$x'x - x'\frac{1}{n}Px = x'\left(I - \frac{1}{n}P\right)x \Rightarrow B = I - \frac{1}{n}P$. To solve part (d), $B^2 = BB = \left(I - \frac{1}{n}P\right)\left(I - \frac{1}{n}P\right) = (I-A)(I-A) = I-A-A+A^2 = I-A-A+A = I-A = I-\frac{1}{n}P = B$. Therefore, matrix B is idempotent. Since B is idempotent, then $tr(B) = tr(I-A) = tr(I)-tr(A) = rank(I)-rank(A) = n-1$. By using theorem 2 on page 484 of the text book, we have ns^2/σ^2 is $\chi^2(n-1)$. To solve part (e),

$$AB = \left(\frac{1}{n}P\right)\left(I - \frac{1}{n}P\right) = \frac{1}{n}P - \frac{1}{n}\left(\frac{1}{n}\right)PP =$$

$$\frac{1}{n}P - \frac{1}{n}\left(\frac{1}{n}\right)\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix} =$$

$$\frac{1}{n}P-\frac{1}{n}\left(\frac{1}{n}\right)\begin{pmatrix} n & n & n & \cdots & n \\ n & n & n & \cdots & n \\ n & n & n & \cdots & n \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ n & n & n & \cdots & n \\ n & n & n & \cdots & n \end{pmatrix}=\frac{1}{n}P-\frac{1}{n}P=0.$$

14.34 Short Review

$\rho=\beta\frac{\sigma_x}{\sigma_y}$. Testing $H_0:\rho=0$ is the same as testing $H_0:\beta=0$. For the LRT, $\begin{pmatrix} x \\ y \end{pmatrix}\sim$ bivariate normal(μ,Σ). The parameters are $\mu_1,\mu_2,\sigma_1,\sigma_2,\rho$. The distribution is

$$\frac{1}{2\pi|\Sigma|^{\frac{1}{2}}}\exp\left\{-\frac{1}{2}(x,y)^T\Sigma^{-1}\begin{pmatrix} x \\ y \end{pmatrix}\right\}.$$

Under LRT, $\rho=0$. $W:\widehat{\mu}_1=\bar{x},\widehat{\mu}_2=\bar{y},\widehat{\sigma}_1=s_1^2,\widehat{\sigma}_2=s_2^2$. $\Omega:\widehat{\mu}_1=\bar{x},\widehat{\mu}_2=\bar{y},\widehat{\sigma}_1=s_1^2,\widehat{\sigma}_2=s_2^2$ and $\widehat{\rho}=r=\frac{s_{xy}}{s_xs_y}$. Then, $\lambda=\frac{\widehat{L}(W)}{\widehat{L}(\Omega)}=c^*(1-r^2)^{\frac{n}{2}}$. $\lambda\le\lambda_0\Rightarrow(1-r^2)\le c^*\Rightarrow|r|\ge k$. The LRT is a function of r.

$$T=\frac{r}{\sqrt{\frac{1-r^2}{n-2}}}=\frac{bd}{\left(\frac{\sum(y_i-\widehat{y}_i)^2}{n-2}\right)^{\frac{1}{2}}}\sim t(n-2)$$

where $d=\sum(x_i-\bar{x})^2$, and $b=\widehat{\beta}$. It can be shown that $\sum(y_i-\bar{y})^2=\sum(y_i-\widehat{y}_i)^2+\sum(\widehat{y}_i-\bar{y})^2=\sum(y_i-\widehat{y}_i)^2+nb^2x_x^2$ where $s_x^2=\frac{1}{n}\sum(x_i-\bar{x})^2$. And note that $1-r^2=1-\frac{s_{xy}^2}{s_x^2s_y^2}=1-b^2\frac{s_x^2}{s_y^2}$ because $b=\widehat{\beta}=\frac{s_{xy}}{s_x^2}\Rightarrow r^2=\frac{b^2s_x^2}{s_y^2}=\frac{\sum(\widehat{y}_i-\bar{y})^2}{\sum(y_i-\bar{y})^2}$. $100r^2$ is the percentage of the variation in the y that is explained by the regression. Testing $H_0:\rho=\rho_0$ can only be done for asymptotically for large n. $r\sim N\left(\rho,\frac{1}{n}\sigma_r^2\right)$, where σ_r is a function of ρ.

$$\frac{r-\rho_0}{\sqrt{\frac{\widehat{\sigma}_r}{\sqrt{n}}}}\sim N(0,1)$$

but does not tend to the normal distribution fast enough. The function

$$\frac{1}{2}\log\left(\frac{1+r}{1-r}\right)\sim N\left[\frac{1}{2}\log\left(\frac{1+\rho_0}{1-\rho_0}\right),\frac{1}{n-3}\right]$$

tends to the normal distribution faster.

$$z=\frac{\frac{1}{2}\log\left(\frac{1+r}{1-r}\right)-\frac{1}{2}\log\left(\frac{1+\rho_0}{1-\rho_0}\right)}{\sqrt{\frac{1}{n-3}}}\sim N(0,1).$$

14.35 Distributions of Quadratic Forms

1. If $z\sim N(0,1)$, then $z^2\sim\chi^2(1)$.

2. If $x_i \sim N(\mu_i, \sigma_i^2)$, $i = 1, 2, ..., n$ then $\sum_{i=1}^{n} \left(\frac{x_i - \mu_i}{\sigma_i}\right)^2 \sim \chi^2(n)$.

3. If $\underline{x} \sim N(\underline{\mu}, \Sigma)$, then $Q = (\underline{x} - \underline{\mu})^T \Sigma^{-1} (\underline{x} - \underline{\mu}) \sim \chi^2(n)$.

4. Let $Q = x^T A x$, where the matrix A is positive semi-definite and symmetric. Let $x_1, x_2, ..., x_n$ be iid $N(0, \sigma^2)$. Then $Q/\sigma^2 \sim \chi^2(r)$ iff A is idempotent of rank r.

5. If $x_1, x_2, ..., x_n$ are iid $N(0, \sigma^2)$ then $Q_1 = x^T A x$ and $Q_2 = x^T B x$ are independent iff $AB = 0$.

6. Cochran's Theorem: Let $x_1, x_2, ..., x_n$ be iid $N(0, \sigma^2)$ and $Q = x^T x = x^T A_1 x + x^T A_2 x + \cdots + x^T A_k x = Q_1 + Q_2 + \cdots + Q_k$ where A_i is symmetric with rank r_i. Then, Q_i/σ^2 is $\chi^2(r_i)$ and is independent of $Q_1, ..., Q_{i-1}, Q_{i+1}, ..., Q_k$ iff $\sum_{j=1}^{k} r_j = n$.

14.36 Non-Parametric Methods

1. x is a continuous random variable.

2. No fixed distribution is assumed for x.

3. Some weak set of assumptions are going to be made.

4. Robust tests and estimators.

5. In general, the power of the tests are going to be lower compared to tests based on specific distributions.

6. Exact values of x_i's are not going to be used. *Orderings or ranks* are going to be used. Thus, there will be a loss of information.

Suppose the random variable x has a distribution function $F(x) = P(X \leq x)$ where $f(x)\,dx$ is the density. What is the distribution of $y = F(x)$? Let $y = F(x)$. $\frac{dy}{dx} = f(x) \Rightarrow f(x)\,dx = 1\,dy, 0 < y < 1. y = F(x) \sim U(0, 1)$. If $x_1, x_2, ..., x_n$ is a random sample, then $F(x_1), F(x_2), ..., F(x_n)$ is a random sample from a uniform distribution. If $y_1 < y_2 < \cdots < y_n$ is the ordered sample, then $F(y_1), F(y_2), ..., F(y_n)$ is an ordered sample from $U(0, 1)$. Let $w_i = F(y_i), i = 1, 2, ..., n$. Then, $w_1, w_2, ..., w_n$ is an ordered sample from $U(0, 1)$. Then $h(w) = n!, 0 < w_1 < w_2 < \cdots < w_n < 1$. The distribution of w_r is $f_{w_r}(w) = \frac{n!}{(r-1)!(n-r)!} w^{r-1}(1 - w)^{n-r}, 0 < w < 1$.

We can find $E(w_r)$ using the beta distribution. $E(w_{r+1} - w_r) = \frac{r+1}{n+1} - \frac{r}{n+1} = \frac{1}{n+1}$. $u_r = w_r - w_{r-1}, r = 2, 3, ..., n$ and $u_1 = w_1$ and $u_{n+1} = 1 - w_n$. So, the ordered random sample is dividing up the density in $(n + 1)$ sections with the same expected value $\frac{1}{n+1}$. $E[F(y_r)] = \frac{r}{n+1}$. Estimate the $\left(\frac{r}{n+1}\right)$ 100th percentile of x. It will be y_r. Estimation of $\xi p \ni F(\xi p) = p$. ξp is the 100pth percentile of the distribution of x. $x_1, x_2, ..., x_n$ is the random sample from this distribution. Let $y_1 < y_2 < \cdots < y_n$ be the ordered sample. Let $k \ni E[F(y_k)] = p$. What k satisfies it? $E[F(y_k)] = \frac{k}{n+1}$, $\frac{k}{n+1} = p \Rightarrow k = (n + 1)p$. Then, we say $\widehat{\xi_p} = y_k$, where $k = p(n + 1)$.

Example: Estimate the median $\xi_{\frac{1}{2}}$ in a sample of size 15. $k = \frac{1}{2}(15 + 1) = 8 \Rightarrow y_8 = \widehat{\xi_{\frac{1}{2}}}$ is the estimator. If $n = 16$, then $k = \frac{1}{2}(17) = 8.5 \Rightarrow \widehat{\xi_{\frac{1}{2}}} = \frac{y_8 + y_9}{2}$. Estimate the 80-th percentile, $p = 0.80$. $k = (0.80)17 = 13.6$. Take the weighted average of y_{13} and y_{14}. $\widehat{\xi_{0.80}} = 0.60 y_{14} + 0.40 y_{13}$. If $x \sim N(\mu, \sigma^2)$, then solve $h(\widehat{\mu}, \widehat{\sigma}, x) = 0.80$ for x where $\phi(x) = P(X \leq x) = h(\mu, \sigma, x)$.

14.36.1 Estimating ξ_p

If $k = (n + 1)p$ then $\widehat{\xi_p} = y_k$ where $y_1 < y_2 < \cdots < y_n$ is the ordered sample. To find the confidence interval of ξ_p is the same as finding $P(y_i < \xi_p < y_j)$. Let u equal to the number of $(x_1, x_2, ..., x_n) < \xi_p$. Then, $u \sim Bin(p, n)$. $P(y_i < \xi_p < y_j) = P(i \leq u \leq j - 1) = \sum_{u=i}^{j-1} \binom{n}{u} p^u q^{n-u} = \theta$. (y_i, y_j) is the 100θ%

confidence interval of ξ_p. For a given θ, finding (i,j) is what is normally done. If $k=(n+1)p$, then center the confidence interval at y_k. Go symmetric to both sides at y_k and find $(i,j) \ni P(y_i < \xi_p < y_j)$ is close to θ.

Example: $n=19$. Find the confidence interval of the median. $p=\frac{1}{2}$ and $(n+1)p=10$. $\widehat{\xi}_{\frac{1}{2}} = y_{10}$.

To find (i,j) for large n, $1-\alpha = P(y_i < \xi < y_j) = P(i \le u \le j-1) = P\left(\frac{i-0.50-np}{\sqrt{npq}} < \frac{u-np}{\sqrt{npq}} \le \frac{j-1+0.50-np}{\sqrt{npq}}\right) = 1-\alpha$. We also want the confidence interval to be symmetric $1-\alpha = P(-z_{\alpha/2} < z < z_{\alpha/2}) \Rightarrow i = np+0.50-z_{\alpha/2}\sqrt{npq}$ and $j = np+0.50+z_{\alpha/2}\sqrt{npq} \Rightarrow (i,j)$ are symmetric about $np+0.50$. For the median, (i,j) are symmetric around k where y_k is the sample median. For $p=q=\frac{1}{2}$, then $i=\frac{n}{2}+0.50-z_{\alpha/2}\frac{\sqrt{n}}{2}$ and $j=\frac{n}{2}+0.50+z_{\alpha/2}\frac{\sqrt{n}}{2} \Rightarrow j=(n+1)-i$.

14.36.2 The Sign Test

To test if ξ is the $(100p_0\%)$-th percentile of x, the following hypotheses are used. $H_0: F(\xi)=p_0$ or $H_0: \xi_{p_0} = \xi$. Suppose that $H_1: \xi_{p_0} < \xi$ and $x_1, x_2, ..., x_n$ is a random sample. Look at $x_1-\xi, x_2-\xi, ..., x_n-\xi$. Then, y is the number of negative signs in the $(x_i-\xi)$'s. Under H_0, $y \sim Bin(n,p_0)$. Under $H_1, y \sim Bin(n,p)$ and $p>p_0$. We can rewrite H_0 and H_1 as $H_0: p=p_0$ versus $H_1: p>p_0$. We reject H_0 if $y \ge c$ where c is such that $\alpha = P(\text{Reject } H_0|H_0) = P(y \ge c|p=p_0) = \sum_{y=c}^{n} \binom{n}{y} p_0^y q^{n-y}$. The statistical power is $k(p) = P(\text{Reject } H_0|H_1) = P(y \ge c|p) = \sum_{y=c}^{n} \binom{n}{y} p^y q^{n-y}, p>p_0$. There is one problem with the sign test. Suppose that $H_0: F(\xi) = \frac{1}{2}$.

```
----X-X-X-X--|---X-X-X-X-X-X------------

VERSUS

---X-X-X-X---|-------X-X-X-X-X-----------
```

The sign test does not consider how far the observations are from ξ.

14.36.3 Wilcoxon Test for the Median

The Wilcoxon Test takes into account the distance that the sign test did not. Assume:

1. x is a continuous random variable.
2. x is symmetric around the median ξ.

The hypotheses tests are $H_0: F(\xi)=\frac{1}{2}$ versus the following three. $H_1: F(\xi) > \frac{1}{2}$, $H_1: F(\xi) < \frac{1}{2}$, or $H_1: F(\xi) \ne \frac{1}{2}$. $x_1, x_2, ..., x_n$ is the random sample. R_i is the rank of the absolute value $|x_i-\xi|$ among the $(|x_1-\xi|, |x_2-\xi|, ..., |x_n-\xi|)$. Define the indicator variable

$$z_i = \begin{cases} 1, & \text{if } x_i - \xi > 0. \\ -1, & \text{if } x_i - \xi < 0. \end{cases}$$

Then, $z_1, z_2, ..., z_n$ are iid and under $H_0: p=\frac{1}{2}$

z_i	$h(z_i)$
-1	p
1	$1-p$

Are R_i and z_i independent? Yes, the rank does not depend on z_i. The test statistic is $W = \sum_{i=1}^n z_i R_i$ which is the sum of the ranks of the positive $(x_i - \xi)$ minus the sum of the ranks of the negative $(x_i - \xi)$. The ranks are $1, 2, ..., n$. Since $z_1, z_2, ..., z_n$ are iid, let $R_j = i$. Replace z_j by z_i. Then $z_j R_j = z_i R_j$. Then, W becomes $W = \sum_{i=1}^n iz_i = \sum_{i=1}^n V_i$ where

V_i	$g(V_i)$
$-i$	p
i	q

$E(W) = 0$ under H_0. $Var(W) = \sum_{i=1}^n Var(V_i) = \sum_{i=1}^n \frac{i^2}{2} + \frac{i^2}{2} = \sum_{i=1}^n i^2 = \frac{n(n+1)(2n+1)}{6} \Rightarrow \sigma_W^2 = \frac{n(n+1)(2n+1)}{6}$. To carry out the test, $z = \frac{w-0}{\sigma_W} \sim N(0,1)$ for large n. Reject for

Note	H_1	Reject If
More Negatives	$F(\xi) > \frac{1}{2}$	$z < -z_\alpha$
More Positives	$F(\xi) < \frac{1}{2}$	$z > z_\alpha$
	$F(\xi) \neq \frac{1}{2}$	$\lvert z\rvert > z_{\alpha/2}$

14.36.4 Median Test

Consider two populations. Let ξ_x be the median of x and ξ_y be the median of y. $x_1, x_2, ..., x_n$ and $y_1, y_2, ..., y_m$ are the random samples. We want to test $H_0 : \xi_x = \xi_y$ versus one of the following alternative hypotheses: $H_1 : \xi_x > \xi_y, H_1 : \xi_x < \xi_y$, or $H_1 : \xi_x \neq \xi_y$. We combine the two samples and find the median of the combined sample. The test statistic is V which is the number of y_j's less than or equal to the combined sample median. We need to find the probability of the x's and the y's falling below the median. $n + m = 2k$ or $2k + 1$.

$$P(V = v) = \frac{\begin{pmatrix} m \\ v \end{pmatrix}\begin{pmatrix} n \\ k-v \end{pmatrix}}{\begin{pmatrix} n+m \\ k \end{pmatrix}}, v = 0, 1, 2..., \min(k, m) \text{ under } H_0.$$

Note	H_1	Reject If
More $y_j's$	$\xi_x > \xi_y$	$V \geq c_1$
More $x_i's$	$\xi_x < \xi_y$	$V \leq c_2$
	$\xi_x \neq \xi_y$	$V > c_1^*$ or $V < c_2^*$

To find c_1 for a fixed α, then

$$\alpha = P(\text{Reject } H_0 | H_0) = P(V \geq c_1 | H_0) = \sum_{v=c_1}^{\min(k,m)} \frac{\begin{pmatrix} m \\ v \end{pmatrix}\begin{pmatrix} n \\ k-v \end{pmatrix}}{\begin{pmatrix} n+m \\ k \end{pmatrix}}.$$

Example: The median test is not always a good test. Consider the following data.

```
--X--X--X--X----Y--Y--Y-----Y--Y--Y----X--X--X--X---
```

These runs have the same median but different distributions. The median test can not test for two different distributions. We must use the *run test* for that.

14.36.5 Run Test

Let F be the distribution function of x and z be that of y. $F(x) = P(X \leq x)$. We want to test $H_0 : F(z) = G(z)$ versus $H_1 : F \neq G$. Let $x_1, x_2, ..., x_m$ and $y_1, y_2, ..., y_n$ be the two random samples. Mix the two samples and order the observations and look for runs of the x's and the y's.

Example: Consider the data $\underline{X}\overline{Y}\underline{XX}\overline{YY}\underline{X}\overline{Y}\underline{XX}\overline{YY}$. $n = m = 6$. The number of runs is 8. R is equal to the number of runs of x's and y's. Reject H_0 : if $R \leq c$. We need the distribution of R under H_0. The number of ways to arrange m x's and n y's is $\frac{(m+n)!}{m!n!} = \left(\begin{array}{c} m+n \\ m \end{array} \right)$. Find $P(R = 2k)$. Suppose that there are k runs of x's and k runs of y's. Then there are $n-1$ partitions of y's. So, there are $\left(\begin{array}{c} n-1 \\ k-1 \end{array} \right)$ groups of y's. For the x's there are $\left(\begin{array}{c} m-1 \\ k-1 \end{array} \right)$ groups of x's. Then,

$$P(R = 2k) = \frac{2 \left(\begin{array}{c} m-1 \\ k-1 \end{array} \right) \left(\begin{array}{c} n-1 \\ k-1 \end{array} \right)}{\left(\begin{array}{c} m+n \\ m \end{array} \right)}.$$

To find $P(R = 2k+1)$, then

$$P(R = 2k+1) = \frac{\left(\begin{array}{c} m-1 \\ k \end{array} \right) \left(\begin{array}{c} n-1 \\ k-1 \end{array} \right) + \left(\begin{array}{c} m-1 \\ k-1 \end{array} \right) \left(\begin{array}{c} n-1 \\ k \end{array} \right)}{\left(\begin{array}{c} m+n \\ m \end{array} \right)}.$$

We want $\alpha = P(R \leq c|H_0)$. So, we find c until we are close to α. $E(R) = \mu_R = \frac{2mn}{m+n} + 1$. $\sigma_R^2 = Var(R) = \frac{(\mu_R - 1)(\mu_R - 2)}{m+n-1}$. For large n and m use $z = \frac{R - \mu_R}{\sigma_R} \to N(0,1)$. Calculate the mean by the formula

$$\frac{1}{\left(\begin{array}{c} m+n \\ m \end{array} \right)} \sum 2k2 \left(\begin{array}{c} m-1 \\ k-1 \end{array} \right) \left(\begin{array}{c} n-1 \\ k-1 \end{array} \right) + \sum \cdots$$

Another use of the run test is for independence and randomness. $x_1, x_2, ..., x_s$ is the random sample. Let L = low and H = high.

1. Too many runs of L and H means a trend. Order the sample. Check if an observation is in the lower half or not. Give L to the observation if in the lower half. So, our sample would be $\underbrace{x_1}_{L}, \underbrace{x_2}_{L}, \underbrace{x_3}_{H}, ..., \underbrace{x_s}_{H}$.

2. Less number of runs means trendy data also. The null hypothesis is that the observations are iid. Reject H_0 if $R \leq c_1$ or if $R \geq c_2$.

14.36.6 Mann-Whitney Wilcoxon Test

The Mann-Whitney Wilcoxon Test tests about two distributions. $H_0 : F(z) = G(z)$. The alternatives can be $H_1 : F(z) > G(z)$, $H_1 : F(z) < G(z)$ or $H_1 : F(z) \neq G(z)$. $x_1, x_2, ..., x_m$ and $y_1, y_2, ..., y_n$ are the two samples.

$$z_{ij} = \begin{cases} 1, & \text{if } x_i < y_j. \\ 0, & \text{otherwise.} \end{cases}$$

There are $m \times n$ z_{ij}'s. The test statistic is $U = \sum_{ij} z_{ij}$. The values of U can be $U = 0, 1, 2, ..., mn$. $E(z_{ij}) = 1P(x_i < y_j) = \frac{1}{2}$ under $H_0 \Rightarrow E(U) = \frac{mn}{2}$. The variance of U can be found. We need $E(U^2) = E[\sum_{ij} z_{ij}^2 + \sum_{j \neq k} z_{ij} z_{ik} + \sum_{i \neq h} z_{ij} z_{hj} + \sum_{i \neq h, j \neq k} z_{ij} z_{hk}] = \frac{mn}{2} = E\left(\sum z_{ij}^2\right)$. For $j \neq k$, $E(z_{ij} z_{ik}) = P(z_{ij} = 1, z_{ik} = 1) = P(y_j > x_i, y_k > x_i) = \frac{1}{3}$. For $i \neq h$, $E(z_{ij} z_{hj}) = \frac{1}{3}$. For $i \neq h$ and $j \neq k$, $E(z_{ij} z_{hk}) = P(z_{ij} = 1, z_{hk} = 1) = P(x_i < y_i, x_h < y_k) = P(x_i < y_i) P(x_h < y_k) = \frac{1}{4}$. $E(U^2) = \frac{mn}{2} + \frac{1}{3} \sum_{j \neq k} + \frac{1}{3} \sum_{i \neq h} + \frac{1}{4} \sum_{i \neq h, j \neq k}$. $\sigma_U^2 = E(U^2) - [E(U)]^2 = mn \frac{(m+n+1)}{12}$. For large m and n use $z = \frac{U - \frac{mn}{2}}{\sigma_U} \to N(0,1)$. If m and n are small, then the y's tend to be larger than the x's. If under H_1, $H_1 : F(z) > G(z) \Rightarrow P(x < c) > P(y < c)$.

H_1	Reject If
$F(z) > G(z)$	$z > z_\alpha$
$F(z) < G(z)$	$z < -z_\alpha$
$F(z) \neq G(z)$	$\lvert z \rvert > z_{\alpha/2}$

Let $h(u, m, n) = P(U = u|m, n)$. Order the x's and the y's together and look at the last observation. Suppose we have $1, 2, ..., m+n$. The last observation can be an x or a y. $u = \sum z_{ij}$. $h(u, m, n) = P(\text{last obs is } x) P(U = u|\text{last obs is } x) + P(\text{last obs is } y) P(U = u|\text{last obs is } y) = \frac{m}{n+m} h(u, m-1, n) + \frac{n}{n+m} h(u-m, m, n-1)$. The boundary conditions are

$$h(u, 0, n) = \begin{cases} 1, & \text{if } u = 0. \\ 0, & \text{otherwise.} \end{cases}$$

$$h(u, m, 0) = \begin{cases} 1, & \text{if } u = 0. \\ 0, & \text{otherwise.} \end{cases}$$

$$h(u, m, n) = \{ \; 0, \quad \text{if } u < 0.$$

So, we have $h(0,1,1) = \frac{1}{2}, h(1,1,1) = \frac{1}{2}, h(0,1,2) = \frac{1}{3}, h(1,1,2) = \frac{1}{3}, h(2,1,2) = \frac{1}{3}$. For example, suppose we have the following sample $YYXYX$. Then, $m = 2, n = 3$ and $u = 1$. Instead of looking at all $m \times n$ pairs, order the combined sample and rank them from 1 to $m \times n$. Let $R_i = Rank(y_{(i)}), i = 1, 2, ..., n$. $U = (R_1 - 1) + (R_2 - 2) + \cdots + (R_i - i) + \cdots + (R_n - n) = \sum_{i=1}^n R_i - \frac{n(n+1)}{2} = T - \frac{n(n+1)}{2}$ where T is the total ranks of the y's.

14.37 Homework and Answers

11.7 Let $y_1 < y_2 < \cdots < y_{100}$ be the order statistics of a random sample of size $n = 100$ from a distribution of the continuous type. Find $i < j$ so that $Pr(y_i < \xi_{0.2} < y_j)$ is about equal to 0.95. $k = (n+1)p = (101)\frac{1}{5} = 20.2 \Rightarrow \widehat{\xi}_{0.2} = \frac{4}{5} y_{20} + \frac{1}{5} y_{21}$. $Pr(y_i < \xi_{0.2} < y_j) = \sum_{w=i}^{j-1} \binom{100}{w} \left(\frac{1}{5}\right)^w \left(\frac{4}{5}\right)^{100-w} = P(i \leq \mu \leq j-1)$. $w \sim bin\left(100, \frac{1}{5}\right)$ with $\mu = (100)\left(\frac{1}{5}\right) = 20$ and $\sigma^2 = (100)\frac{1}{5}\left(\frac{4}{5}\right) = 16$. $z_{0.025} = 1.96$. So, $1 - \alpha = 0.95 \Rightarrow \alpha = 0.05$. We know that $i = np + 0.5 - z_{\alpha/2}\sqrt{npq} = 20 + 0.5 - 1.96\sqrt{16} = 12.66 \approx 13$ and $j = np + 0.5 + z_{\alpha/2}\sqrt{npq} = 20 + 0.5 + 1.96\sqrt{16} = 28.34 \approx 28$.

11.15 Let $x_1, x_2, ..., x_{48}$ be a random sample of size 48 from a distribution that has the distribution function $F(x)$. to test $H_0 : F(41) = \frac{1}{4}$ against $H_1 : F(41) < \frac{1}{4}$ use the statistic y, which is the number of sample observations less than or equal to 41. If the observed value of y is $y \leq 7$, reject H_0 and accept H_1. If $p = F(41)$, find the power function $k(p)$, $0 < p \leq \frac{1}{4}$ of the test. Approximate $\alpha = k\left(\frac{1}{4}\right)$. We wish to test $H_0 : F(41) = \frac{1}{4}$ versus $H_1 : F(41) < \frac{1}{4}$. y is the number of sample observations less than or equal to 41. Accept H_1 if $y \leq 7$. $k(p) = Pr(\text{Reject } H_0|p) = \sum_{y=0}^{7} \binom{48}{y} p^y (1-p)^{48-y}, 0 < p \leq \frac{1}{4}$. y can be approximately $N[np = 48p; np(1-p) = 48p(1-p)]$. Therefore $k(p) = \Phi\left[\frac{7.5 - 48p}{48p(1-p)}\right] - \Phi\left[\frac{-0.5 - 48p}{48p(1-p)}\right]$. Let

$\alpha = k\left(\frac{1}{4}\right)$. Then y can be approximated by $N\left[np = 48\frac{1}{4} = 12, npq = 48\frac{1}{4}\frac{3}{4} = 9\right]$. Then, $\alpha = k\left(\frac{1}{4}\right) = \Phi\left[\frac{7.5-12}{3}\right] - \Phi\left[\frac{-0.5-12}{3}\right] = \Phi(-1.5) - \Phi(-4.17) = 0.0668$.

11.22 A modification of Wilcoxon's statistic that is frequently used is achieved by replacing R_i by $R_i - 1$. That is, use the modification $W_m = \sum_{i=1}^{n} z_i(R_i - 1)$. Show that $W_m/\sqrt{\frac{(n-1)(n)(2n-1)}{6}}$ has a limiting distribution that is $N(0,1)$. $W_m = \sum_{i=1}^{n} z_i(R_i - 1) = \sum_{i=1}^{n}(i-1)Z_i = \sum_{i=1}^{n} v_i$ where

$$v_i = \begin{cases} i-1, & \text{with probability } \frac{1}{2}. \\ -(i-1), & \text{with probability } \frac{1}{2}. \end{cases}$$

$P(z_i = 1) = P(z_j = -1) = \frac{1}{2}$. If H_0 is true, the $E(W) = \sum_{i=1}^{n} E(v_i) = 0$ and $Var(W) = \sum_{i=1}^{n} Var(v_i) = \sum_{i=1}^{n}(i-1)^2 = \frac{(n-1)(n-1+1)(2(n-1)+1)}{6} = \frac{(n-1)n(2n-1)}{6}$. From the text book on pages 511-512, we use Liapounov. Consider $E(|v_i - \mu_i|^3) = (i-1)^3\left(\frac{1}{2}\right) + (i-1)^3\left(\frac{1}{2}\right) = (i-1)^3$. $\sum_{i=1}^{n}(i-1)^3 = \frac{(n-1)^2((n-1)+1)^2}{4} = \frac{(n-1)^2n^2}{4}$. Then, $\sum_{i=1}^{n}\sigma_i^2 = \sum_{i=1}^{n}(i-1)^2 = \frac{(n-1)n(2n-1)}{6}$.

$$\lim_{n\to\infty} \frac{\sum_{i=1}^{n} E(|v_i - \mu_i|^3)}{\sqrt[\frac{3}{2}]{\sum_{i=1}^{n}\sigma_i^2}} = \frac{\frac{(n-1)^2n^2}{4}}{\left(\frac{(n-1)n(2n-1)}{6}\right)^{\frac{3}{2}}}$$

The numerator is of order n^4 and the denominator is of order $\frac{9}{2}$. Therefore, it has a limiting distribution that is $N(0,1)$. And,

$$\frac{\sum_{i=1}^{n} v_i - \sum_{i=1}^{n} u_i}{\sqrt{\sum_{i=1}^{n}\sigma_i^2}} = \frac{W_m}{\sqrt{\frac{(n-1)n(2n-1)}{6}}}.$$

11.32 In the discussion of the run test, let the random variables R_1 and R_2 be, respectively, the number of runs of the values of x and the number of runs of the values of y. Then, $R = R_1 + R_2$. Let the pair (r_1, r_2) of integers be in the space of (R_1, R_2). Then $|r_1 - r_2| \leq 1$. Show that the joint pdf of R_1 and R_2 is

$$f(R_1, R_2) = \begin{cases} 2\binom{m-1}{r_1-1}\binom{n-1}{r_2-1}\Big/\binom{m+n}{m}, & \text{if } r_1 = r_2. \\ \binom{m-1}{r_1-1}\binom{n-1}{r_2-1}\Big/\binom{m+n}{m}, & \text{if } |r_1 - r_2| = 1. \\ 0, & \text{elsewhere.} \end{cases}$$

Show that the marginal pdf of R_1 is

$$f_1(R_1) = \begin{cases} \binom{m-1}{r_1-1}\binom{n+1}{r_1}\Big/\binom{m+n}{m}, & \text{if } r_1 = 1, 2, ..., m. \\ 0, & \text{otherwise.} \end{cases}$$

Find $E(R_1)$. In a similar manner, find $E(R_2)$. Compute $E(R) = E(R_1) + E(R_2)$. R is the total number of runs. R_1 is an integer and is the number of runs of x's. R_2 is the number of runs of y's. If $|r_1 - r_2| \leq 2$, then R_1 and R_2 differ at most by 1. Hence, for the observed values of R_1 and R_2 we have three possibilities: 1) $r_1 = r_2$, 2) $r_1 = r_2 + 1$, and 3) $r_1 = r_2 - 1$. Define the function $G(r_1, r_2)$ which gives the number of ways in which we can obtain r_1 runs of x's runs and r_2 y runs.

$$G(r_1, r_2) = \begin{cases} 0, & \text{for } |r_1 - r_2| > 1. \\ 1, & \text{for } |r_1 - r_2| = 1. \\ 2, & \text{for } r_1 = r_2. \end{cases}$$

If $r_1 = r_2$ then we can arrange r_1 and r_2 runs corresponding runs in two ways and if $|r_1 - r_2| = 1$, this can be done in one way only. From our notes, we already know

$$P(R = 2k) = \frac{2\binom{m-1}{k-1}\binom{n-1}{k-1}}{\binom{m+n}{m}}.$$

So,

$$P(R_1 = r_1, R_2 = r_2) = \frac{2\binom{m-1}{r_1-1}\binom{n-1}{r_2-1}}{\binom{m+n}{m}}.$$

when $r_1 = r_2 = k; r = r_1 + r_2 = 2k$. Note $G(r_1, r_2) = 2$ for $r_1 = r_2$. Also, we can consider $P(R = 2k+1)$ using our notes. For

$$P(R_1 = r_1, R_2 = r_2) = P(R = 2r_2 + 1) =$$

$$\frac{\binom{m-1}{r_2-1}\binom{n-1}{r_2} + \binom{m-1}{r_2}\binom{n-1}{r_2-1}}{\binom{m+n}{m}} = \frac{\binom{m-1}{r_2-1}\binom{n-1}{r_2-1}}{\binom{m+n}{m}}.$$

So, the joint pdf of $P(R_1 = r_1, R_2 = r_2)$ is

$$P(R_1 = r_1, R_2 = r_2) = \begin{cases} \dfrac{2\binom{m-1}{r_1-1}\binom{n-1}{r_2-1}}{\binom{m+n}{m}}, & \text{if } r_1 = r_2. \\ \dfrac{\binom{m-1}{r_1-1}\binom{n-1}{r_2-1}}{\binom{m+n}{m}}, & \text{if } |r_1 - r_2| = 1. \\ 0, & \text{otherwise.} \end{cases}$$

To find the marginals.

$$P(R_1 = r_1) = \sum_{r_2=1}^{n} P(R_1 = r_1, R_2 = r_2) =$$

$$\sum_{r_2=1}^{n} \frac{2\binom{m-1}{r_1-1}\binom{n-1}{r_2-1}}{\binom{m+n}{m}} + \sum_{r_2=1}^{n} \frac{\binom{m-1}{r_1-1}\binom{n-1}{r_2-1}}{\binom{m+n}{m}} + \sum_{r_2=1}^{n} \frac{\binom{m-1}{r_1-1}\binom{n-1}{r_2-1}}{\binom{m+n}{m}} =$$

$$\frac{\binom{m-1}{r_1-1}}{\binom{m+n}{m}}(n-1)!\left[\frac{2}{(r_1-1)!(n-r_1)!} + \frac{1}{(r_1-1)!(n-r_1+1)!} + \frac{1}{r_1!(n-r_1-1)!}\right] =$$

$$\frac{\binom{m-1}{r_1-1}\binom{n+1}{r_1}}{\binom{m+n}{m}}.$$

which is the marginal pdf of R_1. To find the expected value of R_1,

$$E(R_1) = \sum_{r_1=1}^{m} r_1 \frac{\binom{m-1}{r_1-1}\binom{n+1}{r_2}}{\binom{m+n}{m}} = (n+1)\sum_{r_1=1}^{m} \frac{\binom{m-1}{r_1-1}\binom{n+1}{r_2}}{\binom{m+n}{m}} =$$

$$\frac{(n+1)}{\binom{m+n}{m}}\binom{m+n-1}{m-1} = \frac{(n+1)}{(m+n)!}m!n!\frac{(m+n-1)!}{(m-1)!n!} = \frac{(n+1)m}{m+n}.$$

In a similar manner, $E(R_2) = \frac{(m+1)n}{m+n}$. Consider $E(R) = E(R_1) + E(R_2) = \frac{(n+1)m}{m+n} + \frac{(m+1)n}{m+n} = \frac{nm+m+mn+n}{m+n} = \frac{2mn+m+n}{m+n}$.

11.35 Show that $V = T - [n(n+1)]/2$. Hint: Let $Y_{(1)} < Y_{(2)} < \cdots < Y_{(n)}$ be the ordered sample statistics of the random sample $y_1, y_2, ..., y_n$. If R_i is the rank of $Y_{(i)}$ in the combined ordered sample, note that $Y_{(i)}$ is greater than $R_i - i$ values of x. T is the sum of the ranks of $Y_1, Y_2, ..., Y_n$ among the $n+m$ items and R_i is the rank of $Y_{(i)}$ in the combined ordered sample. So, $T = \sum_{j=1}^{n} R_j$. We know that $U = \sum_{j=1}^{n}\sum_{i=1}^{m} z_{ij}$ where

$$z_{ij} = \begin{cases} 1, & \text{if } x_i < y_i. \\ 0, & \text{if } x_i > y_j. \end{cases}$$

Define $y_{(i)}$ is greater than $R_i - i$ values of x. Therefore, $U = \sum_{j=1}^{n}(R_j - j) = \sum_{j=1}^{n} R_j - \sum_{j=1}^{n} j = T - \frac{n(n+1)}{2}$.

Chapter 15

Linear Models

Dr. John P. Morgan, Old Dominion University

Statistics 627, Spring 1997

Text used: *Linear Models,* Shayle Searle

Supplemental Textbook: *Matrix Algebra Useful for Statistics,* Shayle Searle

Grading: Your course grade will be based upon a series of homework assignments (approximately eight for the semester), two tests, and a final exam. The assignments will compose 40% of the grade, the tests 15% each, and the final the remaining 30%. The final exam is scheduled for Tuesday, May 6, 3:45-6:45 pm.

Course Outline: We will follow the text fairly closely in covering chapters 1 through 9, though we will omit some sections entirely. This is primarily a theory course, covering the inner workings of the distributions, statistical tests, and estimation procedures learned in Stat 535 and Stat 537. The material is fundamental to a proper understanding of how SAS runs its linear model procedures (e.g. PROC REG and PROC GLM); indeed, you will notice in the SAS manuals that Searle's text is a primary reference. A thorough knowledge of solving linear equations is needed, which is the topic of Chapter 1. Chapter 2 concentrates on the distributions of linear combinations and quadratic forms involving normal random variables. Chapter 3, onward, will examine a myriad of aspects to the general linear model.

15.1 Notation

Notation	Meaning
A'	Represents the transpose of matrix A. This notation is used early in the notes in this context, but is replaced with A^T. More likely, this notation is reserved for denoting a non-central distribution.
A^T	Represents the transpose of matrix A.
$r(A)$	Always means the rank of matrix A. The variable r rarely appears in this chapter. So generally, r is treated as an operator.
$\chi^{2\prime}(n, \lambda)$	Represents a non-central chi-square distribution where λ is the non-centrality parameter
$F'(n_1, n_2, \lambda)$	Represents a non-central F distribution where n_1 is the numerator degrees of freedom, n_2 is the denominator degrees of freedom, and λ is the non-centrality parameter.
$\varrho(A)$	Represents the column space of matrix A.
$\varrho^{\perp}(A)$.	The set of all vectors orthogonal to every vector in $\varrho(A)$.

15.2 Introduction to Vectors and Matrices

An $m \times n$ matrix $A_{m\times n}$ is a rectangular array of numbers with m rows and n columns. If the number in the i-th row and the j-th column is a_{ij} then the matrix is displayed as

$$A = (a_{ij}) = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix}$$

A *column vector* is a matrix with one column.

$$\underline{a}_{m\times 1} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{pmatrix}$$

When the elements are real numbers, we say $a \subseteq \Re^m$, the m-dimensional real space. All vectors and Matrices in this class will be composed of real numbers. In class, we will use upper case letters for Matrices, underlined letters for vectors, and lower case letters without underlines for numbers (scalars). We reserve some letters for often used Matrices and vectors. I_n is an $n \times n$ matrix with 1's on the diagonal and zero elsewhere and is called the *identity matrix.* $J_{m\times n}$ is an $m \times n$ matrix of 1's. $0_{m\times n}$ is an $m \times n$ matrix of 0's. $J_n \equiv J_{n\times n}$ and $0_n \equiv 0_{n\times n}$. $\underline{j}_n$ is an $n \times 1$ vector of 1's which is equal to $J_{n\times 1}$. $\underline{0}_n$ is an $n \times 1$ vector of 0's which is equal to $0_{n\times 1}$.

If $B_1, B_2, ..., B_n$ are Matrices, then

$$
Diag(B_i) = \begin{pmatrix} B_1 & 0 & 0 & \cdots & \cdots \\ 0 & B_2 & 0 & \cdots & \cdots \\ 0 & 0 & B_3 & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ & & & & B_n \end{pmatrix}
$$

We put the B_i's on the diagonal of the matrix, and 0's elsewhere. The *transpose* of a matrix $A_{m\times n}$ is the matrix $A^T_{n\times m}$ given by interchanging the rows and the columns of A.

$$
A^T = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{m1} \\ a_{12} & a_{22} & \cdots & a_{m2} \\ \vdots & \vdots & \vdots & \vdots \\ a_{1n} & a_{2n} & \cdots & a_{mn} \end{pmatrix}
$$

A set of vectors $\underline{a}_1$, $\underline{a}_2$, ..., $\underline{a}_n$ is said to be independent iff $\sum_{i=1}^{n} c_i\underline{a}_i = \underline{0} \Rightarrow c_1 = c_2 = \cdots = c_n = 0$. The *only* linear combination of the $\underline{a}_i$'s producing the $\underline{0}$ vector is that of multiplying every $\underline{a}_i$ by 0. Take for example,

$$
\underline{a}_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \underline{a}_2 = \begin{pmatrix} 0 \\ 2 \\ 1 \end{pmatrix}, \quad \underline{a}_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.
$$

$c_1\underline{a}_1 + c_2\underline{a}_2 + c_3\underline{a}_3 = \underline{0} \Rightarrow c_1 = 0$, $c_1 + 2c_1 + c_3 = 0 \Rightarrow c_2 = 0 \Rightarrow c_1 = c_2 = c_3 = 0$. Hence, $\underline{a}_1, \underline{a}_2$, and $\underline{a}_3$ are independent. Take for example,

$$
\underline{b}_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \underline{b}_2 = \begin{pmatrix} 0 \\ 2 \\ 1 \end{pmatrix}, \quad \underline{b}_3 = \begin{pmatrix} -2 \\ 0 \\ 1 \end{pmatrix}.
$$

Solve simultaneously $c_1 - 2c_3 = 0, c_1 + 2c_2 = 0, c_2 + c_3 = 0$. So, $c_1 - 2c_2 = 0, 2c_2 + 2c_2 = 0, 4c_2 = 0 \Rightarrow c_1 = 2, c_2 = -1 \Rightarrow c_3 = 1 \Rightarrow c_1\underline{b}_1 + c_2\underline{b}_2 + c_3\underline{b}_3 = \underline{0}$ which implies dependence. We will find it useful to think of a matrix $A_{m\times n}$ as an ordered collection of its n column vectors or its m row vectors. The rank of a matrix A, denoted by $r(A)$, is equal to the number of independent columns in A which is also equal to the number of independent rows in A.

Example: Let

$$
B = \begin{pmatrix} 1 & 0 & -2 \\ 1 & 2 & 0 \\ 0 & 1 & 1 \end{pmatrix}
$$

The rank of B is denoted by $r(B) = 2$ which is columns 1 and 2 only, as an example. It could be other combinations, as well. $A_{m\times n}$ is said to have *full row rank* if $r(A) = m$ and *full column rank* if $r(A) = n$. Suppose that we have the matrix $A_{n\times n}$. Then, we have full rank if $r(A) = n$. It is also called *non-singular.* Otherwise the square matrix is called *singular (not full rank).* The rank $r(A) = n$ iff the determinant $|A| \neq 0$. Let $A_{r\times m} = (a_{ij})$ and $B_{m\times s} = (b_{ij})$. We define the product $C_{r\times s} = AB$ by

$$
C = (c_{ij}) = \left(\sum_{h=1}^{m} a_{ih}b_{nj} \right).
$$

Example: Define the following matrices.

$$A_{3\times 2} = \begin{pmatrix} 1 & -1 \\ 1 & 0 \\ 1 & 1 \end{pmatrix}, \quad B_{2\times 4} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & -1 & -2 \end{pmatrix}, \quad C_{3\times 4} = \begin{pmatrix} 0 & -1 & 2 & 3 \\ 1 & 1 & 1 & 1 \\ 2 & 3 & 0 & -1 \end{pmatrix}.$$

In general, for $C = AB, r(C) \leq \min[r(A), r(B)] = 2$. Likewise, a $1 \times n$ vector can be multiplied by an $n \times 1$ vector. Define the vectors

$$\underline{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}, \quad \underline{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}.$$

We can not multiply $\underline{a} \times \underline{b}$. But, we can multiply $\underline{a}^T \underline{b} = \sum_{i=1}^{n} a_i b_j$. The vectors $\underline{a}$ and $\underline{b}$ are *orthogonal* if $\underline{a}^T \underline{b} = 0$. The square matrix $A_{n\times n}$ is *positive definite* iff

1. $\underline{x}^T A \underline{x} \geq 0, \forall \underline{x}$.
2. $\underline{x}^T A \underline{x} = 0 \Rightarrow \underline{x} = \underline{0}$.

If (2) fails to hold true, but (1) holds true then matrix A is *semi-positive definite.* The *trace* of a square matrix is the sum of its diagonal elements: $tr(A_{n\times n} = \sum_{i=1}^{n} a_{ii}$. Also, $tr(A + B) = tr(A) + tr(B)$. Also, $tr(AB) = tr(BA)$ for AB and BA both square. For example A can be a 3×5 matrix and B can be a 5×3 matrix. So, $AB = 3 \times 3$ matrix which is square. $BA = 5 \times 5$ matrix which is square. A square matrix A is *idempotent* if $A^2 = A$. A square matrix A is *orthogonal* if $A^T A = I$. If A is idempotent, then $tr(A) = r(A)$ and $I - A$ is idempotent. The *colum space* of a matrix $A_{m\times n}$ is the set of all vectors that can be written as linear combinations of A. This is also called the *range* of A or the *manifold* of A. It will be denoted by $\varrho(A)$. Likewise, we define the *row space* of A as $\Re(A) = \varrho(A^T)$. By $\varrho^{\perp}(A)$, we mean the set of all vectors orthogonal to every vector in $\varrho(A)$. Likewise, we can define $\Re^{\perp}(A)$.

Example: Define the following matrix.

$$A = \begin{pmatrix} 1 & 0 & -2 \\ 1 & 2 & 0 \\ 0 & 1 & 1 \end{pmatrix}.$$

Then,

$$\begin{pmatrix} 1 \\ 3 \\ 1 \end{pmatrix} \in \varrho(A), \quad \begin{pmatrix} 1 \\ -1 \\ 2 \end{pmatrix} \in \varrho^{\perp}(A), \quad \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \notin \varrho(A) \text{ or } \varrho^{\perp}(A).$$

For any matrix A, $\varrho(A) = \varrho(AA^T)$, and $\Re(A) = \Re(A^T A)$. Hence, $r(A) = r(AA^T) = r(A^T A)$. The following matrix is considered partitioned.

$$B_{4\times 5} = \begin{pmatrix} 1 & 6 & \vdots & 3 & 6 & 0 \\ 3 & 4 & \vdots & 5 & -1 & 0 \\ \cdots & \cdots & \vdots & \cdots & \cdots & \cdots \\ 2 & -1 & \vdots & 8 & 0 & 2 \\ 7 & 0 & \vdots & 9 & 9 & 1 \end{pmatrix} = \begin{pmatrix} B_{11} & \vdots & B_{12} \\ \cdots & \vdots & \cdots \\ B_{21} & \vdots & B_{22} \end{pmatrix}$$

Partitioning can be done in many ways. One advantage is that it can simplify the matrix multiplication. Consider

$$A_{2\times 4} = \begin{pmatrix} 1 & 0 & \vdots & 1 & 1 \\ 0 & 1 & \vdots & 0 & 1 \end{pmatrix}.$$

Then, $A_{2\times 4}B_{4\times 5} =$

$$\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 6 \\ 3 & 4 \end{pmatrix} + \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 2 & -1 \\ 7 & 0 \end{pmatrix} \vdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 3 & 6 & 0 \\ 5 & -1 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 8 & 0 & 2 \\ 9 & 9 & 1 \end{pmatrix}\right] =$$

$$\left[\begin{pmatrix} 1 & 6 \\ 3 & 4 \end{pmatrix} + \begin{pmatrix} 9 & -1 \\ 7 & 0 \end{pmatrix} \vdots \begin{pmatrix} 3 & 6 & 0 \\ 5 & -1 & 0 \end{pmatrix} + \begin{pmatrix} 17 & 9 & 3 \\ 9 & 9 & 1 \end{pmatrix}\right] = \begin{bmatrix} 10 & 5 & \vdots & 20 & 15 & 3 \\ 10 & 4 & \vdots & 14 & 8 & 1 \end{bmatrix}$$

Example: The column space of A, $\varrho(A)$, is the set of all linear combinations of columns of A. For $A_{m\times n}$, partitioned columnwise, $A = (\underline{a}_{1_{m\times 1}} \vdots \underline{a}_{2_{m\times 1}} \vdots \cdots \vdots \underline{a}_{n_{m\times 1}})$, where $\underline{a}_i$ is the i-the column of A. Let

$$\underline{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}.$$

Then,

$$A_{m\times n}\underline{x}_{n\times 1} = (\underline{a}_{1_{m\times 1}} \vdots \underline{a}_{2_{m\times 1}} \vdots \cdots \vdots \underline{a}_{n_{m\times 1}}) \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = x_1\underline{a}_1 + x_2\underline{a}_2 + \cdots + x_n\underline{a}_n$$

which is a member of $\varrho(A)$. In general, $\varrho(A) = \{A\underline{x} : \underline{x} \in \Re^n\}$. For example, let

$$A = \begin{pmatrix} 1 & 0 & -2 \\ 1 & 2 & 0 \\ 0 & 1 & 1 \end{pmatrix}.$$

Then,

$$\varrho(A) = \left\{ x_1 \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} + x_2 \begin{pmatrix} 0 \\ 2 \\ 1 \end{pmatrix} + x_3 \begin{pmatrix} -2 \\ 0 \\ 1 \end{pmatrix} : x_i \in \Re. \right\}$$

We have also demonstrated the general principle that *post multiplication* takes linear combinations of columns. Likewise, *pre-multiplication* of a matrix takes linear combinations of rows. In general, if

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1s} \\ A_{21} & A_{22} & \cdots & A_{2s} \\ \vdots & \vdots & \cdots & \vdots \\ A_{t1} & A_{t2} & \cdots & A_{ts} \end{pmatrix}$$

A partition of matrix A into ts sub-Matrices,

$$B = \begin{pmatrix} B_{11} & B_{12} & \cdots & B_{1q} \\ B_{21} & B_{22} & \cdots & B_{2q} \\ \vdots & \vdots & \cdots & \vdots \\ B_{s1} & B_{s2} & \cdots & B_{sq} \end{pmatrix}.$$

A partition of matrix B into sq sub-Matrices are partitioned so that the number of columns in (A_{ik}) is equal to the number of rows in matrix (B_{kj}), then the product AB is the partitioned matrix $AB = \left(\sum_{k=1}^{s} A_{ik}B_{kj}\right)_{i,j}$. That is, we use regular matrix multiplication, but the elements are the sub-Matrices.

Definition: Projection: Let the matrix $A_{m\times n}$ be some matrix with column space $\varrho(A)$. Then, $\varrho^{\perp}(A)$ is the set of all vectors that are orthogonal to $\varrho(A)$.

Result: If $\underline{z} \in \Re^m$, then $\underline{z}$ can be *uniquely* written as $\underline{z} = \underline{x}+\underline{y}$, where $\underline{x} \in \varrho(A)$, and $\underline{y} \in \varrho^{\perp}(A)$. **Proof:** Suppose $\underline{z} = \underline{x}_1+\underline{y}_1 = \underline{x}_2+\underline{y}_2$ for $\underline{x}_1 \neq \underline{x}_2 \in \varrho(A)$ and $\underline{y}_1 \neq \underline{y}_2 \in \varrho^{\perp}(A)$. Then, $\underline{0} = \underline{z}-\underline{z} = \overbrace{(\underline{x}_1 - \underline{x}_2)}^{\underline{x}_3} + \overbrace{(\underline{y}_1 - \underline{y}_2)}^{\underline{y}_3} = \overbrace{\underline{x}_3}^{\in\varrho(A)} + \overbrace{\underline{y}_3}^{\in\varrho^{\perp}(A)}$. We have $\underline{x}_3 + \underline{y}_3 = 0$ and $\underline{x}_3^T\underline{y}_3 = 0 \Rightarrow \underline{x}_3^T(-\underline{x}_3) = 0 \Rightarrow \underline{x}_3^T\underline{x}_3 = 0 \Rightarrow \underline{x}_3 = \underline{0}$. From that, we can conclude that $\underline{y}_3 = \underline{0} \Rightarrow \underline{x}_1 = \underline{x}_2$ and $\underline{y}_1 = \underline{y}_2$ which implies a contradiction. Call $\underline{x}$ the projection of $\underline{z}$ onto $\varrho(A)$. Call $\underline{y}$ the projection of $\underline{z}$ orthogonal to $\varrho(A)$. FACT: Corresponding to the matrix A, there is a unique matrix P, such that for every $\underline{z} \in \Re^m$, $P\underline{z}$ is the projection of $\underline{z}$ on $\varrho(A)$. We will derive this matrix at the end of Chapter 1 of the text book. We will use two results from linear algebra.

Theorem 0.1: Let the matrix $A_{m\times n}$ imply $\exists P_{m\times m}, Q_{n\times n}$ which are non-singular and

$$P_{m\times m}A_{m\times n}Q_{n\times n} = \begin{pmatrix} D_r & 0 \\ 0 & 0 \end{pmatrix}$$

where D_r is an $r\times r$ diagonal matrix and r is the rank of matrix A. If derived, P and Q can be chosen so that $D_r = I_r$. The proof can be found on page 192 of the reference book to these notes.

Theorem 0.2: Suppose the matrix $A_{n\times n}$ is symmetric and has rank r. This implies there exists a matrix Q that is non-singular such that

$$Q^TAQ = \begin{pmatrix} D_r & 0 \\ 0 & 0 \end{pmatrix}.$$

If desired, Q may be chosen so that

$$D_r = \begin{pmatrix} I_s & 0 \\ 0 & -I_{r-s} \end{pmatrix}_{r\times r}$$

which is called *Lagrange's reduction.* The proof can be found on pages 201-204 of the reference book to these notes.

15.3 Generalized Inverses

These notes come from Section 1.1 of the text book.

Definition: A *generalized inverse* (or g-inverse) of a matrix A is any matrix G which satisfies the property $AGA = A$, even for non-singular Matrices A. We first show that a g-inverse *always* exists. By Theorem 0.1, for any matrix $A_{p\times q}$, there exists the Matrices $P_{p\times p}$ and $Q_{q\times q}$ which are non-singular and

$$PAQ = \begin{pmatrix} D_r & 0 \\ 0 & 0 \end{pmatrix} = \Delta_{p\times q}$$

where D_r is a square, non-singular diagonal $r \times r$ matrix and $r = rank(A)$. Let

$$\Delta^-_{p\times q} = \begin{pmatrix} D_r^{-1} & 0 \\ 0 & 0 \end{pmatrix}$$

and now write $G = Q\Delta^- P$. Then, $AGA = P^{-1}\Delta \overbrace{Q^{-1}Q}^{=I} \Delta^- \overbrace{PP^{-1}}^{=I} \Delta Q^{-1} = P^{-1}\Delta\Delta^-\Delta Q^{-1}$,

$$\Delta\Delta^-\Delta = \begin{pmatrix} D_r & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} D_r^{-1} & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} D_r & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} D_r & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} D_r & 0 \\ 0 & 0 \end{pmatrix}.$$

Then, $P^{-1}\Delta Q^{-1} = A$ because $P^{-1}PAQQ^{-1} = A$. Therefore G as defined, is a g-inverse of A.

Example: Define the following Matrices.

$$A_{3\times 5} = \begin{pmatrix} 1 & 2 & 1 & 1 & 1 \\ 2 & 4 & -1 & 0 & 1 \\ 0 & 2 & 0 & 2 & 4 \end{pmatrix}, \quad P_{3\times 3} = \begin{pmatrix} \frac{1}{3} & \frac{1}{3} & -1 \\ \frac{2}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{2} \end{pmatrix}, \quad Q_{5\times 5} = \begin{pmatrix} 1 & 0 & 0 & \frac{5}{3} & \frac{10}{3} \\ 0 & 0 & 1 & -1 & -2 \\ 0 & 1 & 0 & -\frac{2}{3} & -\frac{1}{3} \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

We can check that

$$PAQ = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}.$$

$$\Delta^-_{5\times 3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$G_{5\times 3} = Q\Delta^- P = \begin{pmatrix} \frac{1}{3} & \frac{1}{3} & -1 \\ 0 & 0 & \frac{1}{2} \\ \frac{2}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Check that $AGA = A$. Next, another method for finding g-inverses will be given. Given a matrix $A_{p\times q}$ of rank r, find any square sub-matrix of r rows and rank r. Let R and S be the permutation Matrices necessary to bring the sub-matrix to the upper left hand corner, i.e.

$$RAS = B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

where B_{11} is the chosen sub-matrix of rank r. Then,

$$G = S\begin{pmatrix} B_{11}^{-1} & 0 \\ 0 & 0 \end{pmatrix}R$$

is a g-inverse of A. **proof:**

$$AGA = AS\begin{pmatrix} B_{11}^{-1} & 0 \\ 0 & 0 \end{pmatrix}RA.$$

FACT: The inverse of a permutation matrix is it's transpose. Note that $RAS = B \Rightarrow A = R^T BS^T$. Then,

$$R^T BS^T S\begin{pmatrix} B_{11}^{-1} & 0 \\ 0 & 0 \end{pmatrix} RR^T BS^T = R^T B\begin{pmatrix} B_{11}^{-1} & 0 \\ 0 & 0 \end{pmatrix} BS^T =$$

$$R^T\begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}\begin{pmatrix} B_{11}^{-1} & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} S^T =$$

$$R^T\begin{pmatrix} I & 0 \\ B_{21}B_{11}^{-1} & 0 \end{pmatrix}\begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} S^T = R^T\begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{21}B_{11}^{-1}B_{12} \end{pmatrix} S^T.$$

Now, show that $B_{22} = B_{21}B_{11}^{-1}B_{12}$.

$$B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \text{ has rank } r.$$

The rows $(B_{21} \ : \ B_{22})$ depend on the rows of $(B_{11} \ : \ B_{12})$. So, there exists a matrix K such that $K \ni: (B_{11} \ : \ B_{12}) = (B_{21} \ : \ B_{22}) \Rightarrow K\, B_{11} = B_{21} \Rightarrow K = B_{21}B_{11}^{-1}$. Also, $K\, B_{12} = B_{22}$. This implies then, $B_{21}B_{11}^{-1}B_{12} = B_{22}$. So, $R^T BS^T = A$ See page 6 of the text book.

15.4 Homework and Answers

Dr. Morgan uses the notation A' to mean the transpose of a matrix in this homework. In the notes and succeeding homework, he uses the notation A^T for the transpose of matrix A.

1. Let the matrix A be given by

$$A = \begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{pmatrix}$$

Do the following.

(a) Determine the rank $r(A)$ of matrix A.

$$\left(\begin{array}{cccc|c} 1 & 2 & 0 & 1 & y_1 \\ -1 & 1 & 2 & 0 & y_2 \\ 0 & 3 & 2 & 1 & y_3 \end{array}\right) \to R_1 + R_2,$$

$$\left(\begin{array}{cccc|c} 1 & 2 & 0 & 1 & y_1 \\ 0 & 3 & 2 & 1 & y_1 + y_2 \\ 0 & 3 & 2 & 1 & y_3 \end{array}\right) \to \frac{1}{3}R_2,$$

$$\left(\begin{array}{cccc|c} 1 & 2 & 0 & 1 & y_1 \\ 0 & 1 & \frac{2}{3} & \frac{1}{3} & \frac{y_1+y_2}{3} \\ 0 & 3 & 2 & 1 & y_3 \end{array}\right) \to -3R_2 + R_3,$$

$$\left(\begin{array}{cccc|c} 1 & 2 & 0 & 1 & y_1 \\ 0 & 1 & \frac{2}{3} & \frac{1}{3} & \frac{y_1+y_2}{3} \\ 0 & 0 & 0 & 0 & y_3 - y_1 - y_2 \end{array}\right) \rightarrow -2R_2 + R_1,$$

$$\left(\begin{array}{cccc|c} 1 & 0 & -\frac{4}{3} & \frac{1}{3} & y_1 - \frac{2}{3}(y_1+y_2) \\ 0 & 1 & \frac{2}{3} & \frac{1}{3} & \frac{y_1+y_2}{3} \\ 0 & 0 & 0 & 0 & y_3 - y_1 - y_2 \end{array}\right)$$

$\Rightarrow$ two independent rows $\Rightarrow r(A) = 2$.

(b) Exhibit $r(A)$ rows of matrix A that are linearly independent, and show explicitly how the remaining rows can be written as linear combinations of those. Rows 1 and 2 are independent. Then, show that both add-up to row 3.

$$(1,\ 2,\ 0,\ 1) + (-1,\ 1,\ 2,\ 0) = (1-1,\ 2+1,\ 0+2,\ 1+0) = (0,\ 3,\ 2,\ 1).$$

(c) Exhibit $r(A)$ columns of matrix A that are linearly independent, and show explicitly how the remaining columns can be written as linear combinations of those.

$$A^T = \begin{pmatrix} 1 & -1 & 0 \\ 2 & 1 & 3 \\ 0 & 2 & 2 \\ 1 & 0 & 1 \end{pmatrix} \rightarrow -2R_1 + R_2,\ \ -1R_1 + R_4,$$

Now the columns are the rows and elimination can be used. I should get 2 rows of zeros.

$$\begin{pmatrix} 1 & -1 & 0 \\ 0 & 3 & 3 \\ 0 & 2 & 2 \\ 0 & 1 & 1 \end{pmatrix} \rightarrow \frac{1}{3}R_2,$$

$$\begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & 1 \\ 0 & 2 & 2 \\ 0 & 1 & 1 \end{pmatrix} \rightarrow R_1 + R_2,$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 2 & 2 \\ 0 & 1 & 1 \end{pmatrix} \rightarrow -2R_2 + R_3,\ \ -R_2 + R_4,$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Going back to the original matrix,

$$\frac{2}{3}C_2 - \frac{4}{3}C_1 = C_3,$$

$$\begin{pmatrix} \frac{4}{3} \\ \\ \frac{2}{3} \\ \\ \frac{6}{3} \end{pmatrix} + \begin{pmatrix} -\frac{4}{3} \\ \\ \frac{4}{3} \\ \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{4}{3} - \frac{4}{3} \\ \\ \frac{2}{3} + \frac{4}{3} \\ \\ \frac{6}{3} - 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 2 \\ 2 \end{pmatrix}$$

$$\frac{1}{3}C_1 + \frac{1}{3}C_2 = C_4,$$

$$\begin{pmatrix} \frac{1}{3} \\ \\ -\frac{1}{3} \\ \\ 0 \end{pmatrix} + \begin{pmatrix} \frac{2}{3} \\ \\ \frac{1}{3} \\ \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{3} + \frac{2}{3} \\ \\ -\frac{1}{3} + \frac{1}{3} \\ \\ 0 + 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

(d) Find $A'A$. Show explicitly that it has the same row space of A.

$$A'A = \begin{pmatrix} 1 & -1 & 0 \\ 2 & 1 & 3 \\ 0 & 2 & 2 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{pmatrix} = \begin{pmatrix} 1+1+0 & 2-1+0 & 0-2+0 & 1+0+0 \\ 2-1+0 & 4+1+9 & 0+2+6 & 2+0+3 \\ 0-2+0 & 0+2+6 & 0+4+4 & 0+0+2 \\ 1+0+0 & 2+0+3 & 0+0+2 & 1+0+1 \end{pmatrix} =$$

$$\begin{pmatrix} 2 & 1 & -2 & 1 \\ 1 & 14 & 8 & 5 \\ -2 & 8 & 8 & 2 \\ 1 & 5 & 2 & 2 \end{pmatrix}.$$

Observing matrix A,

$$R_1 - R_2 = (1,\ 2,\ 0,\ 1) + (1,\ -1,\ -2,\ 0) = (2,\ 1,\ -2,\ 1)$$

which is row 1 in matrix $A'A$. Also,

$$5R_1 + 4R_2 = (5,\ 10,\ 0,\ 5) + (-4,\ 4,\ 8,\ 0) = (1,\ 14,\ 8,\ 5)$$

which is row 2 in matrix $A'A$.

$$2R_1 + 4R_2 = (2,\ 4,\ 0,\ 2) + (-4,\ 4,\ 8,\ 0) = (-2,\ 8,\ 8,\ 2)$$

which is row 3 of matrix $A'A$.

$$2R_1 + R_2 = (2,\ 4,\ 0,\ 2) + (-1,\ 1,\ 2,\ 0) = (1,\ 5,\ 2,\ 2)$$

which is row 4 of matrix $A'A$. If I show that $A'A$ has rank 2 and rows 1 and 2 are independent, then matrix A and matrix $A'A$ have the same rank. Given that and the computations above, it can be concluded that $A'A$ and A have the same row space.

$$\begin{pmatrix} 2 & 1 & -2 & 1 \\ 1 & 14 & 8 & 5 \\ -2 & 8 & 8 & 2 \\ 1 & 5 & 2 & 2 \end{pmatrix} \rightarrow -2R_2 + R_1,\ \ R_1 + R_3,\ \ -2R_4 + R_1,$$

$$\begin{pmatrix} 2 & 1 & -2 & 1 \\ 0 & -27 & -18 & -9 \\ 0 & 9 & 6 & 3 \\ 0 & -9 & -6 & -3 \end{pmatrix} \rightarrow 3R_3 + R_2,\ \ -3R_4 + R_2,$$

$$\begin{pmatrix} 2 & 1 & -2 & 1 \\ 0 & -27 & -18 & -9 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \to 27R_1 + R_2,$$

$$\begin{pmatrix} 49 & 0 & -72 & 18 \\ 0 & -27 & -18 & -9 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$\Rightarrow$ there are 2 independent rows. Thus, $r(A'A) = 2$.

(e) Find AA'. Show explicitly that it has the same column space of A.

$$AA' = \begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{pmatrix} \begin{pmatrix} 1 & -1 & 0 \\ 2 & 1 & 3 \\ 0 & 2 & 2 \\ 1 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1+4+0+1 & -1+2+0+0 & 0+6+0+1 \\ -1+2+0+0 & 1+1+4+0 & 0+3+4+0 \\ 0+6+0+1 & 0+3+4+0 & 0+9+4+1 \end{pmatrix} =$$

$$\begin{pmatrix} 6 & 1 & 7 \\ 1 & 6 & 7 \\ 7 & 7 & 14 \end{pmatrix}$$

Observing matrix A,

$$\frac{4}{3}C_1 + \frac{7}{3}C_2 = \begin{pmatrix} \frac{4}{3} \\ -\frac{4}{3} \\ 0 \end{pmatrix} + \begin{pmatrix} \frac{14}{3} \\ \frac{7}{3} \\ 7 \end{pmatrix} = \begin{pmatrix} 6 \\ 1 \\ 7 \end{pmatrix} \text{ which is column 1 of } AA'.$$

$$-\frac{11}{3}C_1 + \frac{7}{3}C_2 = \begin{pmatrix} -\frac{11}{3} \\ \frac{11}{3} \\ 0 \end{pmatrix} + \begin{pmatrix} \frac{14}{3} \\ \frac{7}{3} \\ 7 \end{pmatrix} = \begin{pmatrix} 1 \\ 6 \\ 7 \end{pmatrix} \text{ which is column 2 of } AA'.$$

$$-\frac{7}{3}C_1 + \frac{14}{3}C_2 = \begin{pmatrix} -\frac{7}{3} \\ \frac{7}{3} \\ 0 \end{pmatrix} + \begin{pmatrix} \frac{28}{3} \\ \frac{14}{3} \\ 14 \end{pmatrix} = \begin{pmatrix} 7 \\ 7 \\ 14 \end{pmatrix} \text{ which is column 3 of matrix } AA'.$$

$$-7C_1 + 14C_4 = \begin{pmatrix} -7 \\ 70 \end{pmatrix} + \begin{pmatrix} 14 \\ 0 \\ 14 \end{pmatrix} = \begin{pmatrix} 7 \\ 7 \\ 14 \end{pmatrix} \text{ which is column 3 of matrix } AA'.$$

If it is shown that AA' has a column rank of 2, then it is shown that AA' has the same column space as A.

$$\begin{pmatrix} 6 & 1 & 7 \\ 1 & 6 & 7 \\ 7 & 7 & 14 \end{pmatrix} \to -6R_2 + R_1,\ -7R_1 + 6R_3$$

$$\begin{pmatrix} 6 & 1 & 7 \\ 0 & -35 & -35 \\ 0 & 35 & 35 \end{pmatrix} \to R_2 + R_3$$

$$\begin{pmatrix} 6 & 1 & 7 \\ 0 & -35 & -35 \\ 0 & 0 & 0 \end{pmatrix} \to$$

$$\begin{pmatrix} 6 & 1 & 7 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix} \to R_1 - R_2$$

$$\begin{pmatrix} 6 & 0 & 6 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix} \Rightarrow$$

There are 2 independent rows. The rows are the same as the columns. Thus, the rank is 2.

(f) Find the vector space orthogonal to the column space of matrix A, by exhibiting a basis for that space. The column space basis has the form $(-y_3 \quad -y_3 \;\; y_3)$. So, a basis is $(-1 \quad -1 \;\; 1) = \underline{a}^T$.

$$(-1 \quad -1 \;\; 1)\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} = -1 + 1 + 0 = 0.$$

$$(-1 \quad -1 \;\; 1)\begin{pmatrix} 2 \\ 1 \\ 3 \end{pmatrix} = -2 - 1 + 3 = 0.$$

$$(-1 \quad -1 \;\; 1)\begin{pmatrix} 0 \\ 2 \\ 2 \end{pmatrix} = 0 - 2 + 2 = 0.$$

$$(-1 \quad -1 \;\; 1)\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = -1 + 0 + 1 = 0.$$

Therefore $(-1 \quad -1 \;\; 1)$ is orthogonal.

(g) Exhibit a vector that is neither in the column space of matrix A nor in the orthogonal space found in (f). Write your vector as the sum of two vectors, one in each of those spaces. The orthogonal vector is $(-1 \quad -1 \;\; 1)$. The column space used in (c) is $(-1 \quad -1 \;\; 0)$ and $(2 \;\; 1 \;\; 3)$. Then, $(-1 \quad -1 \;\; 1) + (1 \quad -1 \;\; 0) = (0 \quad -2 \;\; 1)$ which is neither orthogonal nor in the column space.

2. B is a $2 \times n$ matrix. If you pre-multiply B by

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

what is the effect on B? Suppose matrix C is $n \times 2$ and you post-multiply by that matrix?

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} & b_{13} & \cdots & b_{1n} \\ b_{21} & b_{22} & b_{23} & \cdots & b_{2n} \end{pmatrix} =$$

$$\begin{pmatrix} 0+b_{21} & 0+b_{22} & 0+b_{23} & \cdots & 0+b_{2n} \\ b_{11}+0 & b_{12}+0 & b_{13}+0 & \cdots & b_{1n}+0 \end{pmatrix}$$

The effect of pre-multiplying B by the matrix interchanges row 1 with row 2 — row 1 becomes two 2 and row 2 becomes row 1.

$$\begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \\ c_{31} & c_{32} \\ \vdots & \vdots \\ c_{n1} & c_{n2} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0+c_{12} & c_{11}+0 \\ 0+c_{22} & c_{21}+0 \\ 0+c_{32} & c_{31}+0 \\ \vdots & \vdots \\ 0+c_{n2} & c_{n1}+0 \end{pmatrix}$$

Post-multiplying C interchanges the columns. Column 1 becomes column 2 and column 2 becomes column 1.

3. D is the matrix

$$\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

You want to form the product AD where A is the matrix in (1).

(a) Do so directly.

$$\begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} =$$

$$\begin{pmatrix} 1+0+0+1 & 0+2+0+0 & 1+0+0+1 & 0+2+0+0 \\ -1+0+0+0 & 0+1+2+0 & -1+0+0+0 & 0+1+2+0 \\ 0+0+0+1 & 0+3+2+0 & 0+0+0+1 & 0+3+2+0 \end{pmatrix} =$$

$$\begin{pmatrix} 2 & 2 & 2 & 2 \\ -1 & 3 & -1 & 3 \\ 1 & 5 & 1 & 5 \end{pmatrix}$$

(b) Choose partitions that make the multiplication simple, then perform the multiplication again, displaying the products of the partitions in your work.

$$\left(\begin{array}{cc|cc} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{array}\right) \left(\begin{array}{cc|cc} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ \hline 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{array}\right) =$$

$$\left(\begin{array}{rr} 1 & 2 \\ -1 & 1 \\ 0 & 3 \end{array}\right)\left(\begin{array}{rr} 1 & 0 \\ 0 & 1 \end{array}\right)+\left(\begin{array}{rr} 0 & 1 \\ 2 & 0 \\ 2 & 1 \end{array}\right)\left(\begin{array}{rr} 0 & 1 \\ 1 & 0 \end{array}\right)\Bigg|\left(\begin{array}{rr} 1 & 2 \\ -1 & 1 \\ 0 & 3 \end{array}\right)\left(\begin{array}{rr} 1 & 0 \\ 0 & 1 \end{array}\right)+\left(\begin{array}{rr} 0 & 1 \\ 2 & 0 \\ 2 & 1 \end{array}\right)\left(\begin{array}{rr} 0 & 1 \\ 1 & 0 \end{array}\right)=$$

$$\left(\begin{array}{rr} 1 & 2 \\ -1 & 1 \\ 0 & 3 \end{array}\right)+\left(\begin{array}{rr} 1 & 0 \\ 0 & 2 \\ 1 & 2 \end{array}\right)\Bigg|\left(\begin{array}{rr} 1 & 2 \\ -1 & 1 \\ 0 & 3 \end{array}\right)+\left(\begin{array}{rr} 1 & 0 \\ 0 & 2 \\ 1 & 2 \end{array}\right)=$$

$$\left(\begin{array}{rr|rr} 2 & 2 & 2 & 2 \\ -1 & 3 & -1 & 3 \\ 1 & 5 & 1 & 5 \end{array}\right).$$

15.5 Solving Linear Equations

We consider the linear equations $A_{m\times n}\underline{x}_{n\times 1} = \underline{y}_{m\times 1}$ where A is a known matrix, $\underline{x}$ is an unknown vector and $\underline{y}$ is a known vector.

Definition: The linear equations $A_{m\times n}\underline{x}_{n\times 1} = \underline{y}_{m\times 1}$ are *consistent* iff every linear relationship among the rows of A also hold among the corresponding elements of $\underline{y}$. That is, $\underline{\ell}^T A = 0^T \Rightarrow \underline{\ell}^T \underline{y} = 0$. $\underline{\ell}^T$ is the relationship to reduce A to zeros.

Result: $\underline{\ell}^T A = 0^T \Rightarrow \underline{\ell}^T \underline{y} = 0$ iff $\exists \underline{m} : A\underline{m} = \underline{y}$. Note that $A\underline{x} = \underline{y}$, so $\underline{m}$ is a solution. **proof:** Suppose $\exists \underline{m} : A\underline{m} : A\underline{m} = \underline{y}$. Let $\underline{\ell} : \underline{\ell}^T A = \underline{0}^T$ be given. Then, $\underline{\ell}^T \underline{y} = \overbrace{\underline{\ell}^T A}^{=\underline{0}^T}\underline{m} = \underline{0}^T\underline{m} = 0$. Suppose $\underline{\ell}^T A = \underline{0}^T \Rightarrow \underline{\ell}^T \underline{y} = 0$. Let $A_{m\times n}$ and let r be LIN columns of A ($r \le m$). Then, $\exists \underline{\ell}_i, i = 1, 2, ..., m-r$, such $\underline{\ell}_i^T \underline{\ell}_j = 0$ for $i \neq j$ and $\underline{\ell}_i^T A = 0^T$ for $i = 1, 2, ..., m-r$. These are an orthogonal basis for $\varrho^{\perp}(A)$. Hence, the $\underline{\ell}_i$ and any r LIN columns from matrix A form a set of m independent m vectors. Hence $\underline{y}$ is dependent on this set. But, $\underline{\ell}_i^T \underline{y} = 0$. That is, $\underline{y}$ is orthogonal to the $\underline{\ell}_i$'s. Hence, $\underline{y}$ depends only on the columns of A. Then, $\underline{y} \in \varrho(A) \Rightarrow \exists \underline{m} : A\underline{m} = \underline{y}$, where we are post-multiplying by some vector.

Theorem 1.1: Given that $\underline{x} = G\underline{y}$ is a solution of $A\underline{x} = \underline{y}$ for every $\underline{y}$ such that $A\underline{x} = \underline{y}$ are consistent iff G is a g-inverse of A. **proof:** Write $A_{m\times n} = (\underline{a}_1, \underline{a}_2, ..., \underline{a}_n)$. Note that $A\underline{x}_j = \underline{a}_j$ are consistent for each j. Take

$$\underline{x}_j = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix}$$

So by assumption, $G\underline{a}_j$ is a solution. Therefore, $AG\underline{a}_j = \underline{a}_j, j = 1, 2, ..., m \Rightarrow AG\underline{a}_1$, $AG\underline{a}_2$, ..., $AG\underline{a}_n$, ($\underline{a}_1$, $\underline{a}_2$, ..., $\underline{a}_n$) $= A \Rightarrow AGA = A \Rightarrow G$ is a g-inverse of A. Now, let G be such that $AGA = A$. For $\underline{y}$ such $A\underline{x} = \underline{y}$ are consistent, $\exists \underline{m}$ such $A\underline{m} = \underline{y} \Rightarrow AGA\underline{m} = AG\underline{y} \Rightarrow A\underline{m} = AG\underline{y} \Rightarrow \underline{y} = A(G\underline{y}) \Rightarrow G\underline{y}$ is a solution to $A\underline{x} = \underline{y}$.

Theorem 1.2: All solutions to the consistent equations $A\underline{x} = \underline{y}$ are generated by $G\underline{y} + (GA - I)\underline{z}$, where $\underline{z}$ is arbitrary and G is any g-inverse of A. **proof:** Let $\underline{x}^*$ be any particular solution of $A\underline{x} = \underline{y}$. We must show that there is some $\underline{z}$, say $\underline{z}^*$ such that $\underline{x}^* = G\underline{y} + (GA - I)\underline{z}^*$. Take $\underline{z}^* = (GA - I)\underline{x}^*$. Then, $G\underline{y} + (GA - I)\underline{z}^* =$

$$G\underline{y}+(GA-I)(GA-I)\underline{x}^* = G\underline{y}+(G\overbrace{AGA}^{=A}-GA-GA+I)\underline{x}^* = G\underline{y}+(I-GA)\underline{x}^* = G\underline{y}+\underline{x}^*-G\overbrace{A\underline{x}^*}^{=\underline{y}} = \underline{x}^*.$$

Lemma 1.1: Let the rank of matrix A, $r(A)=r$ and G be any g-inverse of A. Let q equal to the number of columns of A and $H=GA$. Then, $H_{q\times q}$ and $I-H$ are both idempotent, $r(H)=r$, and $r(I-H)=q-r$. **proof:** $H^2=HH=GAGA=GA=H$. Also, $(I-H)(I-H)=I-H-H+H=I-H$. $r(H)=r(GA)\leq r(A)$ and $r(H)\geq r(AH)=r(AGA)=r(A)$. $r(H)=r(A)$. A known fact for $r(I-H)=tr(I-H)=tr(I)-tr(H)=q-r(H)=q-r$. Recall that for any idempotent matrix $B_j, r(B)=tr(B)$. Now that we have all the solutions to $A\underline{x}=\underline{y}$, how may LIN solutions are there?

Theorem 1.3: When the matrix A is of rank r and has q columns, the number of LIN solutions to the consistent equations $A\underline{x}=\underline{y}$ is

1. $q-r$ if $\underline{y}$ is null ($\underline{0}$).
2. $q-r+1$ if $\underline{y}$ is non-null.

proof: Write $H=GA$ where G is a g-inverse of matrix A. Recall that *all* solutions to $A\underline{x}=\underline{y}$ are $\underline{x}=G\underline{y}+(H-I)\underline{z}$. Since, the rank $r(H-I)=q-r$, we can find $\underline{x}_i=(H-I)\underline{z}_i, i=1,2,....,q-r$ such that the $\underline{x}_i$ are independent. (The notation used here does not intend to imply that x_i is related to X).

1. Consider $\underline{y}=\underline{0}$. Then, This implies $G\underline{y}$ is null which implies that $\underline{x}_i, i=1,2,...,q-r$ are a full set of $q-r$ LIN solutions.
2. Consider $\underline{y}$ is non-null. Let $\underline{x}_0=G\underline{y}$. We first show that $\underline{x}_i, i=0,1,2,...,q-r$ are LIN. For if this is true, then $\underline{x}_0, \underline{x}_0+\underline{x}_1, \underline{x}_0+\underline{x}_2,...,\underline{x}_0+\underline{x}_{q-r}$ are a LIN set since the transformation is non-singular. So, suppose that this is not true. Then, $\exists\lambda_i, i=0,1,2,...,q-r$ that are not all zero with $\lambda_0\neq 0$ subject to $\sum_{i=0}^{q-r}\lambda_i\underline{x}_i=\underline{0}\Rightarrow \lambda_0 G\underline{y}+\sum_{i=1}^{q-r}\lambda_i(H-I)\underline{z}_i=\underline{0}$. Pre-multiply by A to get $\lambda_0\overbrace{AG\underline{y}}^{=\underline{y}}+\sum_{i=1}^{q-r}\lambda_i\overbrace{A(H-I)}^{=0}z_i \Rightarrow \lambda_0\underline{y}=\underline{0}$ which implies a contradiction. Note that $A(H-I)=A(GA-I)=AGA-A=0$. Hence, $\underline{x}_0, \underline{x}_0+\underline{x}_1, \underline{x}_0+\underline{x}_2,...,\underline{x}_0+\underline{x}_{q-r}$ are LIN and are easily seen to be solutions to $A\underline{x}=\underline{y}$.

Given linearly independent solutions, other solutions are found as follow: $A\underline{x}=\underline{y}$ are consistent and LIN solutions are $\underline{x}_1,\underline{x}_2,...,\underline{x}_s$.

1. If $\underline{y}=\underline{0}, \sum_i\lambda_i\underline{x}_i$ is a solution for all $\lambda_1,\lambda_2,....$
2. If $\underline{y}\neq\underline{0}, \sum_i\lambda_i\underline{x}_i$ is a solution iff $\sum_i\lambda_i=1$.

In the study of linear models, we will be concerned with linear combinations of the elements of a solution to a set of equations. In particular, for what vector $\underline{k}$ is $\underline{k}^T\underline{x}$ *invariant* to the choice of $\underline{x}$? The term "invariant" is used here to mean that it does not change the vector $\underline{x}$.

Theorem 1.4: $\underline{k}^T\underline{x}$ is invariant to the choice of the solution to the consistent equations $A\underline{x}=\underline{y}$ iff $\underline{k}^TH=\underline{k}^T$, where $H=GA$ and G is a g-inverse of A. **proof:** Let G be any g-inverse of matrix A. All solutions to $A\underline{x}=\underline{y}$ are $G\underline{y}+(H-I)\underline{z}$ where $\underline{z}$ is arbitrary. Hence, the possible values of $\underline{k}^T\underline{x}$ as we look at different solutions of $\underline{x}$ are $\underline{k}^T[G\underline{y}+(H-I)\underline{z}]$ which is independent of $\underline{z}$ iff $\underline{k}^T(H-I)\underline{z}=0,\forall\underline{z}$ iff $\underline{k}^TH\underline{z}=\underline{k}^T\underline{z},\forall\underline{z}$ iff $\underline{k}^TH=\underline{k}^T$. Take $\underline{z}$ equal to each unit vector $\underline{e}_i$ where

$$\underline{e}_i=\begin{pmatrix}0\\0\\0\\\vdots\\1\\0\\0\end{pmatrix}.$$

Corollary 1.1: $\underline{k}^T\underline{x}$ is invariant to the choice of solution $A\underline{x} = \underline{y}$ iff $\underline{k}^T = \underline{w}^T H$, for some $\underline{w}$. $\underline{k}^T \in \Re(H)$) iff $\underline{k}^T = \underline{\ell}^T A$ for some $\underline{\ell}$. $\underline{k}^T \in \Re(A)$. Need Theorem 1.4 for the proof. **proof:** Suppose $\underline{k}^T\underline{x}$ is invariant. By Theorem 1.4, $\underline{k}^T H = \underline{k}^T \Rightarrow \underline{k}^T = \underline{w}H$. Suppose $\underline{k}^T = \underline{w}^T H \Rightarrow \underline{k}^T H = \underline{w}^T HH = \underline{w}^T H = \underline{k}^T \Rightarrow \underline{k}^T\underline{x}$ is invariant. Suppose $\underline{k}^T\underline{x}$ is invariant. Then, $\underline{k}^T H = \underline{k}^T \Rightarrow \underline{k}^T = \underline{k}^T H = \underline{k}^T GA = \underline{\ell}^T A$ where $\underline{\ell}^T = \underline{k}^T G$. Suppose $\underline{k}^T = \underline{\ell}^T A$ for some $\underline{\ell} \Rightarrow \underline{k}^T H = \underline{\ell}^T AH = \underline{\ell}^T AGA = \underline{\ell}^T A = \underline{k}^T \Rightarrow \underline{k}^T\underline{x}$ is invariant.

Corollary 1.2: There are exactly $r = r(A)$ LIN vectors $\underline{k}$ such that $\underline{k}^T\underline{x}$ is invariant to the choice of solution to $A\underline{x} = \underline{y}$. **proof:** Using Corollary 1.1, $\underline{k}^T \in \Re(A)$, and $r(A) = r \Rightarrow \Re(A)$ contains exactly r LIN vectors.

Example: Define the following Matrices.

$$A = \begin{pmatrix} 1 & 2 & 1 & 1 & 1 \\ 2 & 4 & -1 & 0 & 1 \\ 0 & 2 & 0 & 2 & 4 \end{pmatrix} \quad G = \begin{pmatrix} \frac{1}{3} & \frac{1}{3} & -1 \\ 0 & 0 & \frac{1}{2} \\ \frac{2}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Consider $A_{3\times 5}\underline{x}_{5\times 1} = \begin{pmatrix} 2 \\ -2 \\ 4 \end{pmatrix} = \underline{y}$ One solution is

$$G\underline{y} = \begin{pmatrix} \frac{1}{3} & \frac{1}{3} & -1 \\ 0 & 0 & \frac{1}{2} \\ \frac{2}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 2 \\ -2 \\ 4 \end{pmatrix} = \begin{pmatrix} -4 \\ 2 \\ 2 \\ 0 \\ 0 \end{pmatrix}$$

Now let's find all the solutions. There should be $q - r + 1 = 5 - 3 + 1 = 3$ LIN solutions.

$$H = GA = \begin{pmatrix} \frac{1}{3} & \frac{1}{3} & -1 \\ 0 & 0 & \frac{1}{2} \\ \frac{2}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 2 & 1 & 1 & 1 \\ 2 & 4 & -1 & 0 & 1 \\ 0 & 2 & 0 & 2 & 4 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & -\frac{5}{3} & -\frac{10}{3} \\ 0 & 1 & 0 & 1 & 2 \\ 0 & 0 & 1 & \frac{2}{3} & \frac{1}{3} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

are all of the solutions.

$$G\underline{y} + (H - I)\underline{z} = \begin{pmatrix} 4 \\ 2 \\ 2 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & -\frac{5}{3} & -\frac{10}{3} \\ 0 & 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & \frac{2}{3} & \frac{1}{3} \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \\ z_5 \end{pmatrix}.$$

A set of 3 LIN solutions is $G\underline{y}$, $G\underline{y} + \underline{x}_1$, and $G\underline{y}\underline{x}_2$, where $\underline{x}_1, \underline{x}_2$ are independent columns.

$$\lambda_1 \begin{pmatrix} -4 \\ 2 \\ 2 \\ 0 \\ 0 \end{pmatrix}, \ \lambda_2 \begin{pmatrix} -\frac{17}{3} \\ 3 \\ \frac{8}{3} \\ -1 \\ 0 \end{pmatrix}, \ \lambda_3 \begin{pmatrix} -\frac{22}{4} \\ 4 \\ \frac{7}{3} \\ 0 \\ -1 \end{pmatrix}$$

or $\lambda_1, \lambda_2, \lambda_3$ add up to 1. For what vectors $\underline{k}$ will $\underline{k}^T\underline{x}$ be invariant to the solution $\underline{x}$? Just those in $\Re(H)$ or $\Re(A)$. For example, $\underline{k}^T = (0, 1, 3, 3, 3) = R_2 + 3R_3$ of H

$$\underline{k}^T \begin{pmatrix} -4 \\ 2 \\ 2 \\ 0 \\ 0 \end{pmatrix} = 8, \ \underline{k}^T \begin{pmatrix} -\frac{17}{3} \\ 3 \\ \frac{8}{3} \\ -1 \\ 0 \end{pmatrix} = 8, \ \underline{k}^T \begin{pmatrix} -\frac{22}{3} \\ 4 \\ \frac{7}{3} \\ 0 \\ -1 \end{pmatrix} = 8.$$

Note that $\underline{k}^T H = \underline{k}^T$. On the other hand, consider $\underline{k}^T = (1,1,1,1,1)$. Here $\underline{k}^T H = (1,1,1,0,-1) \neq \underline{k}^T$.

$$\underline{k}^T \begin{pmatrix} -4 \\ 2 \\ 2 \\ 0 \\ 0 \end{pmatrix} = 0, \ \underline{k}^T \begin{pmatrix} -\frac{17}{3} \\ 3 \\ \frac{8}{3} \\ -1 \\ 0 \end{pmatrix} = -1, \ \underline{k}^T \begin{pmatrix} -\frac{22}{3} \\ 4 \\ \frac{7}{3} \\ 0 \\ -1 \end{pmatrix} = -2.$$

Therefore, $\underline{k}^T$ is not invariant to the solution $\underline{x}$.

15.6 G-Inverses for Symmetric, Non-Negative Definite Matrices

Skip Sections 3 and 4 in the text book.

Fact: Matrix A is symmetric and non-negative definite iff $A = X^T X$ for some X. We will prove this in Chapter 2 of the text book.

Lemma 1.2: $PX^TX = Q^TX^TX \Rightarrow PX^T = QX^T$. **proof:** $0 = (PX^TX - QX^TX)$, $0 = (PX^TX - QX^TX)(P-Q)^T = 0 = (PX^T - QX^T)(PX^T - QX^T)^T = WW^T$. We have $WW^T = 0 \Rightarrow W = 0 \Rightarrow PX^T - QX^T = 0 \Rightarrow PX^T = QX^T$.

Theorem 1.5: If matrix G is a g-inverse of X^TX, then

1. G^T is also a g-inverse of X^TX.
2. GX^T is a g-inverse of X.
3. XGX^T is invariant to G.
4. XGX^T is symmetric whether G is or not.

proof:

1. $X^TX = X^TXGX^TX$. Transpose both sides to obtain $(X^TX)^T = (X^TXGX^TX)^T \Rightarrow X^TX = X^TXG^TX^TX \Rightarrow A = AG^TA \Rightarrow G^T$ is a g-inverse of X^TX.
2. Apply Lemma 1.2. $\overbrace{X^TXG^T}^{=P} X^TX = X^TX$ and let $Q = I \Rightarrow X^TXG^TX^T = X^T \Rightarrow XGX^TX = X$. GX^T is a g-inverse of X.
3. Let $F \neq G$ be two g-inverses of X^TX. Then by (2), $\overbrace{XF}^{=P} X^TX = \overbrace{XG}^{=Q} X^TX \Rightarrow XFX^T = XGX^T$.
4. Let any g-inverse matrix G, of X^TX be given. Then $S = \frac{1}{2}G + \frac{1}{2}G^T$ is symmetric. By (1), S is a g-inverse of X^TX. Hence by (3), $XGX^T = XSX^T$, and XSX^T are clearly symmetric. The following theorem is a result in projection that is not in the text book.

Theorem 1.6: The matrix which projects onto the column space of X is XGX^T where G is any g-inverse of X^TX. **proof:** Let Y be a matrix such that $\varrho(Y) = \varrho^T(X) \Rightarrow X^TY = 0$. So, any vector $\underline{z}$ may be expressed as $\underline{z} = \underline{x} + \underline{y} = X\underline{\alpha} + Y\underline{\beta} \Rightarrow XGX^T\underline{z} = \overbrace{XGX^TX}^{=X}\underline{\alpha} + \overbrace{XGX^TY}^{=0}\underline{\beta} = X\underline{\alpha} = \underline{x}$ using Theorem 1.5.

15.7 Homework and Answers

1. Recall the matrix

$$A = \begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{pmatrix}$$

from Homework 1. Do the following.

(a) Give an example of a $\underline{y}$ for which the equations $A\underline{x} = \underline{y}$ are *not* consistent.

$$\begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 0 \\ -2 \\ 1 \end{pmatrix} \rightarrow -R_1 - R_2 + R_3 = R_3 \Rightarrow$$

$$\left(\begin{array}{cccc|c} 1 & 2 & 0 & 1 & 0 \\ -1 & 1 & 2 & 0 & -2 \\ 0 & 0 & 0 & 0 & 3 \end{array}\right)$$

The last row can not hold true for any x_1, x_2, x_3, x_4. Therefore, the vector $\begin{pmatrix} 0 \\ -2 \\ 1 \end{pmatrix}$ is inconsistent.

(b) Find a g-inverse of A.

$$m = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} 1 & 2 \\ -1 & 1 \end{pmatrix}$$

Then,

$$\left(\begin{array}{cc|cc} 1 & 2 & 1 & 0 \\ -1 & 1 & 0 & 1 \end{array}\right) \rightarrow R_1 + R_2$$

$$\left(\begin{array}{cc|cc} 1 & 2 & 1 & 0 \\ 0 & 3 & 1 & 1 \end{array}\right) \rightarrow \frac{1}{3}R_2$$

$$\left(\begin{array}{cc|cc} 1 & 2 & 1 & 0 \\ 0 & 1 & \frac{1}{3} & \frac{1}{3} \end{array}\right) \rightarrow -2R_2 + R_1$$

$$\left(\begin{array}{cc|cc} 1 & 0 & \frac{1}{3} & -\frac{2}{3} \\ 0 & 1 & \frac{1}{3} & \frac{1}{3} \end{array}\right) \Rightarrow$$

$$m^{-1} = \begin{pmatrix} \frac{1}{3} & -\frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} \end{pmatrix}$$

$$(m^{-1})^T = \begin{pmatrix} \frac{1}{3} & \frac{1}{3} \\ -\frac{2}{3} & \frac{1}{3} \end{pmatrix}$$

$$G^T = \begin{pmatrix} \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ -\frac{2}{3} & \frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$G = \begin{pmatrix} \frac{1}{3} & -\frac{2}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Proof:

$$AG = \begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{3} & -\frac{2}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{3}+\frac{2}{3}+0+0 & -\frac{2}{3}+\frac{2}{3}+0+0 & 0 \\ -\frac{1}{3}+\frac{1}{3}+0+0 & \frac{2}{3}+\frac{1}{3}+0+0 & 0 \\ 0+1+0+0 & 0+1+0+0 & 0 \end{pmatrix}$$

$$AGA = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{pmatrix} = \begin{pmatrix} 1+0+0 & 2+0+0 & 0+0+0 & 1+0+0 \\ 0-1+0 & 0+1+0 & 0+2+0 & 0+0+0 \\ 1-1+0 & 2+1+0 & 0+2+0 & 1+0+0 \end{pmatrix} =$$

$$\begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{pmatrix} = A.$$

Since $AGA = A \Rightarrow G$ is a g-inverse.

(c) Show that for the $\underline{y}$ found in (a), $AG\underline{y} \neq \underline{y}$.

$$AG\underline{y} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ -2 \\ 1 \end{pmatrix} = \begin{pmatrix} 0+0+0 \\ 0-2+0 \\ 0-2+0 \end{pmatrix} = \begin{pmatrix} 0 \\ -2 \\ -2 \end{pmatrix} \neq \begin{pmatrix} 0 \\ -2 \\ 1 \end{pmatrix} \Rightarrow AG\underline{y} \neq \underline{y}.$$

(d) Find a full set of linearly independent solutions to $A\underline{x} = \underline{0}$. Dr. Morgan recommends finding two columns from $GA - I$ as opposed to this simplistic method.

$$\begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

$$\left(\begin{array}{rrrr|r} 1 & 2 & 0 & 1 & 0 \\ -1 & 1 & 2 & 0 & 0 \\ 0 & 3 & 2 & 1 & 0 \end{array}\right) \to R_1 + R_2$$

$$\left(\begin{array}{rrrr|r} 1 & 2 & 0 & 1 & 0 \\ 0 & 3 & 2 & 1 & 0 \\ 0 & 3 & 2 & 1 & 0 \end{array}\right) \to$$

$$\left(\begin{array}{rrrr|r} 1 & 2 & 0 & 1 & 0 \\ 0 & 3 & 2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{array}\right) \to$$

$$\left(\begin{array}{rrrr|r} 1 & 2 & 0 & 1 & 0 \\ 0 & 1 & \frac{2}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{array}\right) \to -2R_2 + R_1$$

$$\left(\begin{array}{rrrr|r} 1 & 0 & -\frac{4}{3} & \frac{1}{3} & 0 \\ 0 & 1 & \frac{2}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 \end{array}\right).$$

So,

$$\begin{pmatrix} \frac{4}{3}x_3 - \frac{1}{3}x_4 \\ -\frac{2}{3}x_3 - \frac{1}{3}x_4 \\ x_3 \\ x_4 \end{pmatrix} \Rightarrow \begin{pmatrix} \frac{4}{3} \\ -\frac{2}{3} \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} -\frac{1}{3} \\ -\frac{1}{3} \\ 0 \\ 1 \end{pmatrix} \text{ are solutions.}$$

(e) Find a full set of linearly independent solutions to

$$A\underline{x} = \begin{pmatrix} 3 \\ -2 \\ 1 \end{pmatrix}.$$

$$G\underline{y} = \begin{pmatrix} \frac{1}{3} & -\frac{2}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 3 \\ -2 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 + \frac{4}{3} + 0 \\ 1 - \frac{2}{3} + 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{7}{3} \\ \frac{1}{3} \\ 0 \\ 0 \end{pmatrix} \text{ is one solution.}$$

$$GA - I = \begin{pmatrix} \frac{1}{3} & -\frac{2}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} =$$

$$\begin{pmatrix} \frac{1}{3}+\frac{2}{3}+0 & \frac{2}{3}-\frac{2}{3}+0 & 0-\frac{4}{3}+0 & \frac{1}{3}+0+0 \\ \frac{1}{3}-\frac{1}{3}+0 & \frac{2}{3}+\frac{1}{3}+0 & 0+\frac{2}{3}+0 & \frac{1}{3}+0+0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} =$$

$$\begin{pmatrix} 1 & 0 & -\frac{4}{3} & \frac{1}{3} \\ 0 & 1 & \frac{2}{3} & \frac{1}{3} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & -\frac{4}{3} & \frac{1}{3} \\ 0 & 0 & \frac{2}{3} & \frac{1}{3} \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

$$G\underline{y}+(GA-I)\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{7}{3} \\ \frac{1}{3} \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} -\frac{4}{3} \\ \frac{2}{3} \\ -1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ -1 \\ 0 \end{pmatrix} \text{ is the second solution.}$$

$$G\underline{y}+(GA-I)\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{7}{3} \\ \frac{1}{3} \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} \frac{1}{3} \\ \frac{1}{3} \\ 0 \\ -1 \end{pmatrix} = \begin{pmatrix} \frac{8}{3} \\ \frac{2}{3} \\ 0 \\ -1 \end{pmatrix} \text{ is the third solution.}$$

(f) Write an expression for the set of all solutions to the equations in (e).

$$G\underline{y}+(GA-I)\underline{z} = \begin{pmatrix} \frac{7}{3} \\ \frac{1}{3} \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & -\frac{4}{3} & \frac{1}{3} \\ 0 & 0 & \frac{2}{3} & \frac{1}{3} \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \underline{z} = \begin{pmatrix} \frac{7}{3} \\ \frac{1}{3} \\ 0 \\ 0 \end{pmatrix} + z_3 \begin{pmatrix} -\frac{4}{3} \\ \frac{2}{3} \\ -1 \\ 0 \end{pmatrix} + z_4 \begin{pmatrix} \frac{1}{3} \\ \frac{1}{3} \\ 0 \\ -1 \end{pmatrix}$$

(g) In Homework 1, you found the rank r(A) rows of A which are linearly independent. Taking $\underline{K}'$ to be each of these, show explicitly that $\underline{k}'\underline{x}$ is invariant to the solution $\underline{x}$ found in (f). $\underline{K}^T$ of row 1 is

$$\underline{K}^T\underline{X} = (1\ \ 2\ \ 0\ \ 1)\begin{pmatrix} \frac{7}{3} \\ \frac{1}{3} \\ 0 \\ 0 \end{pmatrix} = \frac{7}{3}+\frac{2}{3}+0+0 = 3.$$

$$\underline{K}^T\underline{X} = (1\ \ 2\ \ 0\ \ 1)\begin{pmatrix} 1 \\ 1 \\ -1 \\ 0 \end{pmatrix} = 1+2+0+0 = 3.$$

$$\underline{K}^T\underline{X} = (1\ \ 2\ \ 0\ \ 1)\begin{pmatrix} \frac{8}{3} \\ \frac{2}{3} \\ 0 \\ -1 \end{pmatrix} = \frac{8}{3}+\frac{4}{3}+0-\frac{3}{3} = 3 \Rightarrow \underline{K}^T \text{ is invariant.}$$

For $\underline{K}^T$ of row 2,

$$\underline{K}^T\underline{X} = (-1\ \ 1\ \ 2\ \ 0)\begin{pmatrix} \frac{7}{3} \\ \frac{1}{3} \\ 0 \\ 0 \end{pmatrix} = -\frac{7}{3}+\frac{1}{3}+0+0 = -2.$$

$$\underline{K}^T\underline{X} = (-1\ \ 1\ \ 2\ \ 0)\begin{pmatrix} 1 \\ 1 \\ -1 \\ 0 \end{pmatrix} = -1+1-2+0 = -2.$$

$$\underline{K}^T\underline{X} = (-1\ \ 1\ \ 2\ \ 0)\begin{pmatrix} \frac{8}{3} \\ \frac{2}{3} \\ 0 \\ -1 \end{pmatrix} = -\frac{8}{3}+\frac{2}{3}+0-0 = -2 \Rightarrow \underline{K}^T \text{ is invariant.}$$

2. Still using matrix A as given in (1), do the following. Need to find a g-inverse for A^TA.

$$A^TA = \begin{pmatrix} 1 & -1 & 0 \\ 2 & 1 & 3 \\ 0 & 2 & 2 \\ 1 & 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{pmatrix} = \begin{pmatrix} 1+1+0 & 2-1+0 & 0-2+0 & 1+0+0 \\ 2-1+0 & 4+1+9 & 0+2+6 & 2+0+3 \\ 0-2+0 & 0+2+6 & 0+4+4 & 0+0+2 \\ 1+0+0 & 2+0+3 & 0+0+2 & 1+0+1 \end{pmatrix} =$$

$$\begin{pmatrix} 2 & 1 & -2 & 1 \\ 1 & 14 & 8 & 5 \\ -2 & 8 & 8 & 2 \\ 1 & 5 & 2 & 2 \end{pmatrix}$$

Using the first two rows,

$$\left(\begin{array}{cc|cc} 2 & 1 & 1 & 0 \\ 1 & 14 & 0 & 1 \end{array}\right) \to \left(\begin{array}{cc|cc} 1 & \frac{1}{2} & \frac{1}{2} & 0 \\ 1 & 14 & 0 & 1 \end{array}\right) \to \left(\begin{array}{cc|cc} 1 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{27}{2} & -\frac{1}{2} & 1 \end{array}\right) \to \left(\begin{array}{cc|cc} 1 & 0 & \frac{28}{54} & -\frac{1}{27} \\ 0 & \frac{27}{2} & -\frac{1}{2} & 1 \end{array}\right) \to$$

$$\left(\begin{array}{cc|cc} 1 & 0 & \frac{28}{54} & -\frac{1}{27} \\ 0 & 1 & -\frac{1}{27} & \frac{2}{27} \end{array}\right) \Rightarrow (M^{-1})^T = \begin{pmatrix} \frac{28}{54} & -\frac{1}{27} \\ -\frac{1}{27} & \frac{2}{27} \end{pmatrix} \Rightarrow$$

$$G^T = \begin{pmatrix} \frac{28}{54} & -\frac{1}{27} & 0 & 0 \\ -\frac{1}{27} & \frac{2}{27} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \Rightarrow G = \begin{pmatrix} \frac{28}{54} & -\frac{1}{27} & 0 & 0 \\ -\frac{1}{27} & \frac{2}{27} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

(a) Find the matrix which projects onto the column space of A. Call this matrix P.

$$P = AGA^T = \begin{pmatrix} 1 & 2 & 0 & 1 \\ -1 & 1 & 2 & 0 \\ 0 & 3 & 2 & 1 \end{pmatrix} \begin{pmatrix} \frac{28}{54} & -\frac{1}{27} & 0 & 0 \\ -\frac{1}{27} & \frac{2}{27} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} A^T =$$

$$\begin{pmatrix} \frac{28}{54} - \frac{2}{27} & -\frac{1}{27} + \frac{4}{27} & 0 & 0 \\ -\frac{28}{54} - \frac{1}{27} & \frac{1}{27} + \frac{2}{27} & 0 & 0 \\ 0 - \frac{3}{27} & 0 + \frac{6}{27} & 0 & 0 \end{pmatrix} A^T = \begin{pmatrix} \frac{24}{54} & \frac{3}{27} & 0 & 0 \\ -\frac{30}{54} & \frac{3}{27} & 0 & 0 \\ -\frac{3}{27} & \frac{6}{27} & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & -1 & 0 \\ 2 & 1 & 3 \\ 0 & 2 & 2 \\ 1 & 0 & 1 \end{pmatrix} =$$

$$\begin{pmatrix} \frac{24}{54} + \frac{6}{27} & -\frac{24}{54} + \frac{3}{27} & \frac{9}{27} \\ \frac{30}{54} + \frac{6}{27} & \frac{30}{54} + \frac{3}{27} & \frac{9}{27} \\ -\frac{3}{27} + \frac{12}{27} & \frac{3}{27} + \frac{6}{27} & \frac{18}{27} \end{pmatrix} = \begin{pmatrix} \frac{36}{54} & -\frac{18}{54} & \frac{9}{27} \\ -\frac{18}{54} & \frac{36}{54} & \frac{9}{27} \\ \frac{9}{27} & \frac{9}{27} & \frac{18}{27} \end{pmatrix} =$$

$$\frac{1}{3} \begin{pmatrix} 2 & -1 & 1 \\ -1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix} = P$$

(b) Evaluate $P\underline{x}$ for the independent columns $\underline{x}$ found in 1(c) of Homework 1. Explain what you see. Columns 1 and 2 are independent. Using column 1,

$$\begin{pmatrix} \frac{36}{54} & -\frac{18}{54} & \frac{9}{27} \\ -\frac{18}{54} & \frac{36}{54} & \frac{9}{27} \\ \frac{9}{27} & \frac{9}{27} & \frac{18}{27} \end{pmatrix} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{36}{54} + \frac{18}{54} + 0 \\ -\frac{18}{54} - \frac{36}{54} + 0 \\ \frac{9}{27} - \frac{9}{27} + 0 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}.$$

Using column 2,

$$\begin{pmatrix} \frac{36}{54} & -\frac{18}{54} & \frac{9}{27} \\ -\frac{18}{54} & \frac{36}{54} & \frac{9}{27} \\ \frac{9}{27} & \frac{9}{27} & \frac{18}{27} \end{pmatrix} \begin{pmatrix} 2 \\ 1 \\ 3 \end{pmatrix} = \begin{pmatrix} \frac{72}{54} - \frac{18}{54} + \frac{27}{27} \\ -\frac{36}{54} - \frac{36}{54} + \frac{27}{27} \\ \frac{18}{27} + \frac{9}{27} + \frac{54}{27} \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ 3 \end{pmatrix}.$$

Since P projects onto $\varrho(A)$, and each of the above vectors is in $\varrho(A)$, $P\underline{x} = \underline{x}$. Indeed, $P\underline{x} = \underline{x}, \forall \underline{x} \in \varrho(A)$.

(c) Evaluate $P\underline{x}$ for the basis vector $\underline{x}$ of $\varrho^{\perp}(A)$ found in 1(f) of Homework 1. Explain what you see.

$$\begin{pmatrix} \frac{36}{54} & -\frac{18}{54} & \frac{9}{27} \\ -\frac{18}{54} & \frac{36}{54} & \frac{9}{27} \\ \frac{9}{27} & \frac{9}{27} & \frac{18}{27} \end{pmatrix} \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix} = \begin{pmatrix} -\frac{36}{54} + \frac{18}{54} + \frac{9}{27} \\ \frac{18}{54} - \frac{36}{54} + \frac{9}{27} \\ -\frac{9}{27} - \frac{9}{27} + \frac{18}{27} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

The basis vector of $\underline{x}$ of $\varrho^{\perp}(A)$ is orthogonal to the matrix P also. It has no projection onto $\varrho(A)$ since it is entirely in $\varrho^{\perp}(A)$.

(d) In 1(g) of Homework 1 you found a vector $\underline{x}$ which was neither in $\varrho(A)$ nor $\varrho^{\perp}(A)$. Evaluate $P\underline{x}$ and $(1-P)\underline{x}$. Do you recognize the results?

$$P\underline{x} = \begin{pmatrix} \frac{36}{54} & -\frac{18}{54} & \frac{9}{27} \\ -\frac{18}{54} & \frac{36}{54} & \frac{9}{27} \\ \frac{9}{27} & \frac{9}{27} & \frac{18}{27} \end{pmatrix} \begin{pmatrix} 0 \\ -2 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 + \frac{36}{54} + \frac{9}{27} \\ 0 - \frac{72}{54} + \frac{9}{27} \\ 0 - \frac{18}{27} + \frac{18}{27} \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}.$$

which is column 1 of matrix A.

$$(I-P)\underline{x} = \left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} \frac{36}{54} & -\frac{18}{54} & \frac{9}{27} \\ -\frac{18}{54} & \frac{36}{54} & \frac{9}{27} \\ \frac{9}{27} & \frac{9}{27} & \frac{18}{27} \end{pmatrix} \right] \underline{x} =$$

$$\begin{pmatrix} \frac{18}{54} & \frac{18}{54} & -\frac{9}{27} \\ \frac{18}{54} & \frac{18}{54} & -\frac{9}{27} \\ -\frac{9}{27} & -\frac{9}{27} & \frac{9}{27} \end{pmatrix} \begin{pmatrix} 0 \\ -2 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 - \frac{36}{54} - \frac{9}{27} \\ 0 - \frac{36}{54} - \frac{9}{27} \\ 0 + \frac{18}{27} + \frac{9}{27} \end{pmatrix} = \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}.$$

These are the parts of $\underline{x}$ which lie in $\varrho(A)$ and $\varrho^{\perp}(A)$, respectively.

3. Prove corollary 1.1 of your class notes. I put this proof in the notes on page 1002.

4. $X_{N\times k} = (x_{ij})$ is a data matrix. The j-th column contains N measurements $x_{1j}, x_{2j}, ..., x_{Nj}$ on the j-th variable (like in a SAS data set). Let $\underline{1}$ be an $N \times 1$ vector of ones. Show that the following statements are true. The matrices look like this.

$$X_{N\times k} = \begin{pmatrix} x_{11} & x_{12} & x_{13} & \cdots & x_{1k} \\ x_{21} & x_{22} & x_{23} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{N1} & x_{N2} & x_{N3} & \cdots & x_{Nk} \end{pmatrix}, \quad \underline{1}_{N\times 1} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

(a) The sample means for the k variables are in the vector $\underline{1}'X/(\underline{1}'\underline{1})$.

$$\underline{1}'X = \left(\sum_{i=1}^{N} x_{i1}, \ \sum_{i=1}^{N} x_{i2}, \ \sum_{i=1}^{N} x_{i3}, \ \cdots \sum_{i=1}^{N} x_{ik} \right),$$

$$\underline{1}'\underline{1} = (1 \ 1 \ 1 \ 1 \ \cdots \ 1) \begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} = 1 + 1 + 1 + \cdots + 1 = N \Rightarrow$$

$$(\underline{1}'X)/(\underline{1}'\underline{1}) = \frac{\left(\sum_{i=1}^{N} x_{i1}, \ \sum_{i=1}^{N} x_{i2}, \ \sum_{i=1}^{N} x_{i3}, \ \cdots \sum_{i=1}^{N} x_{ik} \right)}{N} =$$
$$\frac{1}{N}\sum_{i=1}^{N} x_{i1}, \ \frac{1}{N}\sum_{i=1}^{N} x_{i2}, \ \frac{1}{N}\sum_{i=1}^{N} x_{i3}, \ \cdots \frac{1}{N}\sum_{i=1}^{N} x_{ik}.$$

(b) The matrix of deviations from the sample means is $X - \underline{11}'X/(\underline{1}'\underline{1})$.

$$\underline{11}' = \begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} (1 \ 1 \ 1 \ 1 \ \cdots \ 1) = \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix},$$

$$\underline{11}'X = \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix} \begin{pmatrix} x_{11} & x_{12} & x_{13} & \cdots & x_{1k} \\ x_{21} & x_{22} & x_{23} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{N1} & x_{N2} & x_{N3} & \cdots & x_{Nk} \end{pmatrix} =$$

$$\begin{pmatrix} \sum_{i=1}^{N} x_{i1} & \sum_{i=1}^{N} x_{i2} & \sum_{i=1}^{N} x_{i3} & \cdots & \sum_{i=1}^{N} x_{ik} \\ \sum_{i=1}^{N} x_{i1} & \sum_{i=1}^{N} x_{i2} & \sum_{i=1}^{N} x_{i3} & \cdots & \sum_{i=1}^{N} x_{ik} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum_{i=1}^{N} x_{i1} & \sum_{i=1}^{N} x_{i2} & \sum_{i=1}^{N} x_{i3} & \cdots & \sum_{i=1}^{N} x_{ik} \end{pmatrix}.$$

$$X - \frac{\underline{1}\underline{1}'X}{N} =$$

$$\begin{pmatrix} x_{11} - \frac{1}{N}\sum_{i=1}^N x_{i1} & x_{12} - \frac{1}{N}\sum_{i=1}^N x_{i2} & x_{13} - \frac{1}{N}\sum_{i=1}^N x_{i3} & \cdots & x_{1k} - \frac{1}{N}\sum_{i=1}^N x_{ik} \\ x_{21} - \frac{1}{N}\sum_{i=1}^N x_{i1} & x_{22} - \frac{1}{N}\sum_{i=1}^N x_{i2} & x_{23} - \frac{1}{N}\sum_{i=1}^N x_{i3} & \cdots & x_{2k} - \frac{1}{N}\sum_{i=1}^N x_{ik} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{N1} - \frac{1}{N}\sum_{i=1}^N x_{i1} & x_{N2} - \frac{1}{N}\sum_{i=1}^N x_{i2} & x_{N3} - \frac{1}{N}\sum_{i=1}^N x_{i3} & \cdots & x_{Nk} - \frac{1}{N}\sum_{i=1}^N x_{ik} \end{pmatrix}$$

(c) $(X - \underline{1}\underline{1}'X/(\underline{1}'\underline{1}))'(X - \underline{1}\underline{1}'X/(\underline{1}'\underline{1})) = X'X - X'\underline{1}\underline{1}'X/(\underline{1}'\underline{1})$.

$$\left(\frac{X - \underline{1}\underline{1}'X}{\underline{1}'\underline{1}}\right)^T \left(\frac{X - \underline{1}\underline{1}'X}{\underline{1}'\underline{1}}\right) =$$

$$\begin{pmatrix} x_{11} - \frac{1}{N}\sum_{i=1}^N x_{i1} & x_{21} - \frac{1}{N}\sum_{i=1}^N x_{i1} & x_{31} - \frac{1}{N}\sum_{i=1}^N x_{i1} & \cdots & x_{N1} - \frac{1}{N}\sum_{i=1}^N x_{i1} \\ x_{12} - \frac{1}{N}\sum_{i=1}^N x_{i2} & x_{22} - \frac{1}{N}\sum_{i=1}^N x_{i2} & x_{32} - \frac{1}{N}\sum_{i=1}^N x_{i2} & \cdots & x_{N2} - \frac{1}{N}\sum_{i=1}^N x_{i2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{1k} - \frac{1}{N}\sum_{i=1}^N x_{ik} & x_{2k} - \frac{1}{N}\sum_{i=1}^N x_{ik} & x_{3k} - \frac{1}{N}\sum_{i=1}^N x_{ik} & \cdots & x_{Nk} - \frac{1}{N}\sum_{i=1}^N x_{ik} \end{pmatrix} \times$$

$$\begin{pmatrix} x_{11} - \frac{1}{N}\sum_{i=1}^N x_{i1} & x_{12} - \frac{1}{N}\sum_{i=1}^N x_{i2} & x_{13} - \frac{1}{N}\sum_{i=1}^N x_{i3} & \cdots & x_{1k} - \frac{1}{N}\sum_{i=1}^N x_{ik} \\ x_{21} - \frac{1}{N}\sum_{i=1}^N x_{i1} & x_{22} - \frac{1}{N}\sum_{i=1}^N x_{i2} & x_{23} - \frac{1}{N}\sum_{i=1}^N x_{i3} & \cdots & x_{2k} - \frac{1}{N}\sum_{i=1}^N x_{ik} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{N1} - \frac{1}{N}\sum_{i=1}^N x_{i1} & x_{N2} - \frac{1}{N}\sum_{i=1}^N x_{i2} & x_{N3} - \frac{1}{N}\sum_{i=1}^N x_{i3} & \cdots & x_{Nk} - \frac{1}{N}\sum_{i=1}^N x_{ik} \end{pmatrix} =$$

$$\begin{pmatrix} \sum_{j=1}^N (x_{j1} - \frac{1}{N}\sum_{i=1}^N x_{i1})^2 & \cdots & \cdots \\ \left(x_{12} - \frac{1}{N}\sum_{i=1}^N x_{i2}\right)\left(x_{11} - \frac{1}{N}\sum_{i=1}^N x_{i1}\right) + \left(x_{22} - \frac{1}{N}\sum_{i=1}^N x_{i2}\right)\left(x_{21} - \frac{1}{N}\sum_{i=1}^N x_{i1}\right) + \cdots & \vdots & \cdots \\ \left(x_{1k} - \frac{1}{N}\sum_{i=1}^N x_{ik}\right)\left(x_{11} - \frac{1}{N}\sum_{i=1}^N x_{ik}\right) + \left(x_{2k} - \frac{1}{N}\sum_{i=1}^N x_{ik}\right)\left(x_{21} - \frac{1}{N}\sum_{i=1}^N x_{i1}\right) + \cdots & \cdots & \sum_{j=1}^N \left(x_{jk} - \frac{1}{N}\sum_{i=1}^N x \right. \end{pmatrix}$$

$$X^T X = \begin{pmatrix} x_{11} & x_{21} & \cdots & x_{N1} \\ x_{12} & x_{22} & \cdots & x_{N2} \\ \vdots & \vdots & \vdots & \vdots \\ x_{1k} & x_{2k} & \cdots & x_{Nk} \end{pmatrix} \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{Nk} \end{pmatrix} =$$

$$\begin{pmatrix} \sum_{i=1}^N x_{i1}^2 & x_{11}x_{12} + x_{21}x_{22} + \cdots + x_{N1}x_{N2} & \cdots \\ x_{12}x_{11} + x_{22}x_{21} + \cdots + x_{N2}x_{N1} & \sum_{i=1}^N x_{i2}^2 & \cdots \\ \vdots & \vdots & \vdots \\ x_{1k}x_{11} + x_{2k}x_{21} + \cdots + x_{Nk}x_{N1} & \cdots & \sum_{i=1}^N x_{Nk}^2 \end{pmatrix}$$

$X'\underline{1}\underline{1}'X/(\underline{1}'\underline{1}) =$

$$\frac{1}{N}\begin{pmatrix} x_{11}\sum_{i=1}^N x_{i1} + \cdots + x_{N1}\sum_{i=1}^N x_{i1} & \cdots & x_{11}\sum_{i=1}^N x_{ik} + \cdots + x_{N1}\sum_{i=1}^N x_{ik} \\ x_{12}\sum_{i=1}^N x_{i1} + \cdots + x_{N2}\sum_{i=1}^N x_{i1} & \cdots & x_{12}\sum_{i=1}^N x_{ik} + \cdots + x_{N2}\sum_{i=1}^N x_{ik} \\ \vdots & \vdots & \vdots \\ x_{1k}\sum_{i=1}^N x_{i1} + \cdots + x_{Nk}\sum_{i=1}^N x_{i1} & \cdots & x_{1k}\sum_{i=1}^N x_{ik} + \cdots + x_{Nk}\sum_{i=1}^N x_{ik} \end{pmatrix}$$

$X'X - X'\underline{1}\underline{1}'X/(\underline{1}'\underline{1}) =$

$$\begin{pmatrix} \sum_{i=1}^N x_{i1}^2 - \frac{1}{N}\left(\sum_{i=1}^N x_{i1}\right)^2 & \cdots & \cdots \\ \sum_{i=1}^N x_{i2}x_{i1} - \frac{1}{N}\sum_{i=1}^N x_{i1}\sum_{i=1}^N x_{i2} & \cdots & \cdots \\ \vdots & \vdots & \vdots \\ \sum_{i=1}^N x_{ik}x_{i1} - \frac{1}{N}\sum_{i=1}^N x_{i1}\sum_{i=1}^N x_{ik} & \cdots & \sum_{i=1}^N x_{ik}^2 - \frac{1}{N}\left(\sum_{i=1}^N x_{ik}\right)^2 \end{pmatrix}$$

Does this equal to $(X - \underline{1}\underline{1}'X/(\underline{1}'\underline{1}))'(X - \underline{1}\underline{1}'X/(\underline{1}'\underline{1}))$?

$$\sum_{i=1}^N x_{i1}^2 - \frac{1}{N}\left(\sum_{i=1}^N x_{i1}\right)^2 =$$

$$\left(x_{11} - \frac{1}{N}\sum_{i=1}^N x_{i1}\right)^2 + \left(x_{21} - \frac{1}{N}\sum_{i=1}^N x_{i1}\right)^2 + \cdots + \left(x_{N1} - \frac{1}{N}\sum_{i=1}^N x_{i1}\right)^2 =$$

$$x_{11}^2 - \frac{2}{N}x_{11}\sum_{i=1}^N x_{i1} + \frac{1}{N^2}\left(\sum_{i=1}^N x_{i1}\right)^2 + x_{21}^2 - \frac{2}{N}x_{21}\sum_{i=1}^N x_{i1} + \frac{1}{N^2}\left(\sum_{i=1}^N x_{i1}\right)^2 =$$

$$\sum_{i=1}^N x_{i1}^2 - \frac{2}{N}\sum_{i=1}^N x_{i1}\sum_{i=1}^N x_{i1} + \frac{1}{N}\left(\sum_{i=1}^N x_{i1}\right)^2 = \sum_{i=1}^N x_{i1}^2 - \frac{1}{N}\left(\sum_{i=1}^N x_{i1}\right)^2.$$

Yes. I presume the other diagonal terms are equal also. I'll show that column 1, row 2 in both matrices are equal.

$$\sum_{i=1}^N x_{i2}x_{i1} - \frac{1}{N}\left(\sum_{i=1}^N x_{i1}\right)\left(\sum_{i=1}^N x_{i2}\right) =$$

$$\left(x_{12}-\frac{1}{N}\sum_{i=1}^{N}x_{i2}\right)\left(x_{11}-\frac{1}{N}\sum_{i=1}^{N}x_{i1}\right)+\left(x_{22}-\frac{1}{N}\sum_{i=1}^{N}x_{i2}\right)\left(x_{21}-\frac{1}{N}\sum_{i=1}^{N}x_{i1}\right)+\cdots$$

working with the RHS:

$$\left(x_{12}x_{11}-x_{12}\frac{1}{N}\sum_{i=1}^{N}x_{i1}-x_{11}\frac{1}{N}\sum_{i=1}^{N}x_{i2}+\frac{1}{N^2}\left(\sum_{i=1}^{N}x_{i2}\right)\left(\sum_{i=1}^{N}x_{i1}\right)\right)+$$
$$\left(x_{22}x_{21}-x_{22}\frac{1}{N}\sum_{i=1}^{N}x_{i1}-x_{21}\frac{1}{N}\sum_{i=1}^{N}x_{i2}+\frac{1}{N^2}\left(\sum_{i=1}^{N}x_{i2}\right)\left(\sum_{i=1}^{N}x_{i1}\right)\right)+\cdots$$

$$\sum_{i=1}^{N}x_{i2}x_{i1}-\frac{1}{N}\sum_{i=1}^{N}x_{i2}\sum_{i=1}^{N}x_{i1}-\frac{1}{N}\sum_{i=1}^{N}x_{i1}\sum_{i=1}^{N}x_{i2}+\frac{1}{N}\sum_{i=1}^{N}x_{i2}\sum_{i=1}^{N}x_{i1}=\sum_{i=1}^{N}x_{i2}x_{i1}-\frac{1}{N}\sum_{i=1}^{N}x_{i1}\sum_{i=1}^{N}x_{i2}.$$

I presume the other non-diagonal elements will equate to each other, also.

(d) Write a scalar formula for the j-th diagonal element of the matrix in (c). What is this?

$$\sum_{i=1}^{N}(x_{ij}-\bar{x}_{\cdot j})^2$$

where x_{ij} is the i-th observation on the j-th variable and $\bar{x}_{\cdot j}$ is the mean of the j-th variable. This looks like the sum of squares due to error.

15.8 Quadratic Forms and Idempotent Matrices

We will cover Sections 2.1-2.3 and Section 2.5 in the text book. Matrix $A_{m\times n}=(a_{ij})$, $\underline{x}_{1\times m}A\underline{y}_{n\times 1}=\sum_{i=1}^{m}\sum_{j=1}^{n}x_iy_ja_{ij}$ is called a *bilinear form.* If $m=n$ and $\underline{x}=\underline{y}$, we have $\sum_{i=1}^{n}\sum_{j=1}^{n}x_ix_ja_{ij}=\sum_{i=1}^{n}x_i^2a_{ii}+\sum^{n}\sum_{i\neq j}^{n}x_ix_ja_{ij}$ is called a *quadratic form.* Let $A_1=\frac{1}{2}(A+A^T)$. Then, $\underline{x}^TA_1\underline{x}=\frac{1}{2}\underline{x}^TA\underline{x}+\frac{1}{2}\underline{x}^TA^T\underline{x}=\frac{1}{2}\underline{x}^TA\underline{x}+\frac{1}{2}\underline{x}^TA\underline{x}=\underline{x}^TA\underline{x}$ and note that A_1 is symmetric. When dealing with a quadratic form, $\underline{x}^TA\underline{x}$, we may assume that A is symmetric. The quadratic form $\underline{x}^TA\underline{x}$ is said to be *positive definite* if $\underline{x}^TA\underline{x}>0$ for every $\underline{x}\neq 0$. Similarly, the matrix A itself is said to be positive definite. $\underline{x}^TA\underline{x}$ is said to be *positive semi-definite* if $\underline{x}^TA\underline{x}\geq 0,\forall\underline{x}$ and $\underline{x}^TA\underline{x}=0$ for at least one $\underline{x}\neq 0$. Likewise, A is said to be positive semi-definite. The quadratic form $\underline{x}^TA\underline{x}$ is *non-negative definite* if it is either positive definite or semi-positive definite and the same for matrix A. Recall Lagrange's reduction. We have matrix A of rank r. Then $\exists Q$, that is non-singular such that

$$Q^TAQ=\begin{pmatrix} I_{r-s} & 0 & 0\\ 0 & -I_s & 0\\ 0 & 0 & 0\end{pmatrix}$$

Let $\underline{y}=Q^{-1}\underline{x}$. Then,

$$\underline{x}^TA\underline{x}=\underline{y}^TQ^TAQ\underline{y}=\underline{y}^T\begin{pmatrix} I_{r-s} & 0 & 0\\ 0 & -I_s & 0\\ 0 & 0 & 0\end{pmatrix}\underline{y}=\sum_{i=1}^{r-s}y_i^2-\sum_{i=r-s+1}^{r}y_i^2.$$

So, A is non-negative definite iff $s=0$ iff

$$Q^TAQ=\begin{pmatrix} I_r & 0\\ 0 & 0\end{pmatrix}$$

iff

$$A = (Q^{-1})^T \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix} Q^{-1} = H^T \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix} H$$

where $H = Q^{-1}$.

$$A = \begin{pmatrix} H_{1_r}^T, & H_{2_{n-r}}^T \end{pmatrix} \begin{pmatrix} I_r & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} H_{1_r} \\ H_{2_{n-r}} \end{pmatrix}$$

where the rank $r(H_1) = r$. Hence, our lemmas.

Lemma 2.1: The symmetric matrix A is non-negative definite iff $\exists H_{r\times n}$ matrix such that $A = H^T H$,where $r = \text{rank}(A)$. If matrix A is non-singular and non-negative definite, then it is positive definite. If matrix A is singular and non-negative definite, then it is positive semi-definite.

Lemma 2.2: Matrix A is symmetric and non-negative definite. Then $\underline{y}^T A\underline{y} = 0$ iff $A\underline{y} = 0$. **proof:** Suppose $A\underline{y} = 0$. Then, $\underline{y}^T A\underline{y} = 0$ iff $A\underline{y} = 0$. **proof:** Suppose $A\underline{y} = 0$. Then, $\underline{y}^T A\underline{y} = 0 \Rightarrow A = H^T H \Rightarrow \underline{y}^T A\underline{y} = \underline{y}^T H^T H\underline{y} = 0 \Rightarrow H\underline{y} = \underline{0} \Rightarrow H^T H\underline{y} = \underline{0} \Rightarrow A\underline{y} = \underline{0}$.

Let $A_{n\times n}$ be symmetric and $B_{n\times n}$ be symmetric and positive definite. Consider the equation $|A - \lambda B| = 0$ which is the determinant and λ is a scalar. Since the coefficient of $\lambda^n = (-1)^n|B| \neq 0$, this is a genuine polynomial of degree n, and hence has n roots.

Lemma 2.3: Matrix A is symmetric and matrix B is symmetric and positive definite. Then $|A - \lambda B| = 0$ has all real roots. **proof:** Suppose that $\alpha + i\beta$ where $i = \sqrt{-1}$ and $\beta \neq 0$ is a root. Then, $|A - (\alpha + i\beta)B| = 0 \Rightarrow \left|\frac{A-\alpha B}{\beta} - iB\right| = 0 \Rightarrow |A_1 - iB| = 0$, $A_1 = \frac{A-\alpha B}{\beta}$ is still symmetric. Now, B is positive definite. So this implies that $B = H^T H$ where H is non-singular which implies that $|(H^T)^{-1}||A_1 - iB||H^{-1}| = 0 \Rightarrow |(H^T)^{-1}A_1H^{-1} - i(H^T)^{-1}BH^{-1}| = 0 \Rightarrow |A_2 - iI| = 0$, $A_2 = (H^T)^{-1}A_1H^{-1}$ is symmetric implies $|A_2^T + iI||A_2 - iI| = 0 \Rightarrow |A_2^T A_2 + I| = 0$ cannot be true because $A_2^T A$ is semi-positive definite and I is positive definite. Hence $|A - \lambda B| = 0$ has roots $\lambda_1, \lambda_2, ..., \lambda_n$ which are real numbers. So, $|A - \lambda B| = (\lambda - \lambda_1)(\lambda - \lambda_2)\cdots(\lambda - \lambda_n)$.

Theorem 2.1: This theorem finds the roots. Matrix A is symmetric and B is symmetric and positive definite. Then, $\exists Q$ such that it is non-singular such

$$Q^T AQ = \begin{pmatrix} \lambda_1 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \lambda_n \end{pmatrix}$$

and $Q^T BQ = I$. **proof:** Consider $A - \lambda_1 B = C$. Then, $|C| = 0$. So, by Lagrange's reduction, there is a matrix D_1 that is non-singular such that

$$D_1^T CD_1 = \begin{pmatrix} 0 & \underline{0}^T \\ \underline{0} & E_1 \end{pmatrix},$$

where E_1 is diagonal. Now let $D_1^T BD_1 = F$ where

$$F = \begin{pmatrix} f_{11} & \underline{f}_{21}^T \\ \underline{f}_{21} & F_{22} \end{pmatrix} \text{ and } f_{11} > 0.$$

Let

$$G_1^T = \begin{pmatrix} \frac{1}{\sqrt{f_{11}}} & \underline{0}^T \\ -\frac{1}{f_{11}}\underline{f}_{21} & I \end{pmatrix}.$$

G_1 is non-singular. Then, it can be verified that

$$G_1^T D_1^T B D_1 G_1 = G_1^T F G = \begin{pmatrix} 1 & \underline{0}^T \\ \underline{0} & B_1 \end{pmatrix},$$

say, and

$$G_1^T D_1^T C D_1 G_1 = \begin{pmatrix} 0 & \underline{0}^T \\ \underline{0} & E_1 \end{pmatrix}$$

Write $Q_1 = D_1 G_1$. Then, Q_1 is non-singular. We have shown that

$$Q_1^T B Q_1 = \begin{pmatrix} 1 & \underline{0}^T \\ \underline{0} & B_1 \end{pmatrix}$$

where B_1 is positive definite and

$$Q_1^T C Q_1 = \begin{pmatrix} 0 & \underline{0}^T \\ \underline{0} & E_1 \end{pmatrix}.$$

So,

$$Q_1^T A Q_1 = Q_1^T C Q_1 + \lambda Q_1^T B Q_1 = \begin{pmatrix} \lambda_1 & \underline{0}^T \\ \underline{0} & A_1 \end{pmatrix}$$

where $A_1 = E_1 + \lambda_1 B_1$ is symmetric. This is the first step for A and B. We repeat this process on A_1 and B_1. Then on A_2 and B_2 etc until the result is established. This is possible provided the roots of A_1 are $\lambda_2, ..., \lambda_n$. Now,

$$Q_1^T(A - \lambda B)Q_1 = \begin{pmatrix} \lambda_1 - \lambda & \underline{0}^T \\ \underline{0} & A_1 - \lambda B_1 \end{pmatrix} \Rightarrow |Q_1^T(A - \lambda B)Q_1| = (\lambda_1 - \lambda)|A_1 - \lambda B_1|$$

which implies that $\lambda_2, ..., \lambda_n$ are the roots of $|A_1 - \lambda B_1|$ since $|Q_1^T(A - \lambda B)Q_1| = |Q_1||Q_1^T||A - \lambda B| = |Q_1|^2 \prod_{i=1}^n (\lambda - \lambda_i)$.

Special Case: Let $B = I$. Then, $|A - \lambda I| = 0$. The roots are called *eigenvalues* of A. $Q^T A Q = D(\lambda_i)$ which is the diagonal matrix of eigenvalues and $Q^T B Q = Q^T Q = I$ i.e. Q is *orthogonal*. For Q^T write Γ. Then, $\Gamma A \Gamma^T = D(\lambda_i)$, $A\Gamma^T = \Gamma^T D(\lambda_i)$, $A\underline{\delta}_i = \underline{\lambda}_i \underline{x}_i$ where $\underline{\delta}_i$ is the i-th row of Γ. $\underline{\delta}_i$ is called the *eigenvector* of A corresponding to the eigenvalue λ_i. We summarize this special case as Corollary 2.1.

Corollary 2.1: Let the matrix $A_{n\times n}$ be symmetric with eigenvalues $\lambda_1, \lambda_2, ..., \lambda_n$. Then, $\exists\, \Gamma$ orthogonal such that $\Gamma A \Gamma^T = D(\lambda_i)$. Furthermore, the rows of Γ are the eigenvectors of A.

We can now attack the question of when a symmetric matrix is idempotent. Again, for $B = I$ and A is symmetric, we have $\Gamma A \Gamma^T = D(\lambda_i) \Rightarrow A = \Gamma^T D(\lambda_i)\Gamma \Rightarrow A^2 = \Gamma^T D(\lambda_i)\Gamma\Gamma^T D(\lambda_i)\Gamma = \Gamma^T D(\lambda_i^2)\Gamma$. So, $A = A^2$ iff $\Gamma^T D(\lambda_i)\Gamma = \Gamma^T D(\lambda_i^2)\Gamma$ iff $D(\lambda_i) = D(\lambda_i^2)$ iff $\lambda_i = 0$ or $\lambda_i = 1$ for every i. Hence, a symmetric matrix is idempotent iff all of its eigenvalues are zero or one. We now prove a more general result.

Lemma 2.4: Matrix A is symmetric and B is symmetric and positive definite. Then, AB is idempotent iff its eigenvalues are all zeros and ones. **proof:** By Lemma 2.1 $B = H^T H$ where H is non-singular. $|AB - \lambda I| = 0$ has roots all zeros and ones iff $|H||AB - \lambda I||H^{-1}| = 0$ has roots of zeros and ones iff $|HABH^{-1} - \lambda HIH^{-1}| = 0$, $|HABH^{-1} - \lambda I| = 0$, $|HAH^T - \lambda I| = 0$ has all roots of zeros and ones iff HAH^T is idempotent iff $HAH^T HAH^T = HAH^T$ iff $AH^T HAH^T H = AH^T H$ iff $AH^T H$ is idempotent iff AB is idempotent.

Lemma 2.5 (Loyne's Lemma): Matrix B is symmetric and idempotent. Matrix Q is symmetric and non-negative definite. If $I - B - Q$ is non-negative definite, then this implies that $BQ = QB = 0$. **proof:** Let $\underline{y} = B\underline{x}$ where $\underline{x}$ is any vector such that $\underline{y}^T B\underline{y} = \underline{x}^T B^T B\underline{y} = \underline{x}^T B\underline{y} = \underline{y}^T\underline{y} \Rightarrow \underline{y}^T(I - B - Q)\underline{y} \geq 0 = \underline{y}^T\underline{y} - \underline{y}^T B\underline{y} - \underline{y}^T Q\underline{y} = -\underline{y}^T Q\underline{y} \Rightarrow \underline{y}^T Q\underline{y}$ must equal to zero. Then by Lemma 2.2, $Q\underline{y} = \underline{0} \Rightarrow QB\underline{x} = \underline{0}\forall\underline{x} \Rightarrow QB = 0 \Rightarrow (QB)^T = 0^T$ i.e. $BQ = 0$.

Theorem 2.2: X_i is an $n \times n$ symmetric matrix of rank $k_i, i = 1, 2, ...p$. $X = \sum_{i=1}^p X_i$ is rank k. Consider the four conditions.

1. X_i is idempotent $\forall i$.
2. $X_i X_j = 0 \forall i \neq j$ i.e. orthogonal to each other.
3. X is idempotent.
4. $k = \sum_{i=1}^p k_i$.

Then, the following pairs of conditions imply all four: (1) and (2); (1) and (3); (2) and (3); (3) and (4); **proof:** Conditions (1) and (2): $X^2 = \left(\sum_{i=1}^p X_i\right)^2 = \sum_{i=1}^p X_i^2 = \sum_{i=1}^p X_i = X \Rightarrow k = r(X) = tr(X) = tr\left(\sum_{i=1}^p X_i\right) = \sum_{i=1}^p tr(X_i) = \sum_{i=1}^p k_i \Rightarrow$ condition (4). Conditions (1) and (3): condition (3) implies that $I - X$ is idempotent and hence non-negative definite; condition (1) implies that $X - X_i - X_j$ is non-negative definite. Thus, $(I - X) + (X - X_i - X_j) = I - X_i - X_j$ is non-negative definite which implies that $X_i X_j = 0$ which implies condition (2) which implies condition (4) above. Consider conditions (2) and (3): Let $\lambda \neq 0$ be a eigenvalue of X_1. Let $\underline{u}$ be the corresponding eigenvector i.e. $\underline{y} = X_1\underline{u} = \lambda\underline{u}$. Then, $X\underline{y} = \left(\sum_{i=1}^n X_i\right)\underline{y} = \sum_{i=2}^p X_i X_1 \underline{u} + X_1\underline{y} = X_1\underline{y} = \lambda X_1\underline{u} = \lambda^2\underline{u} = \lambda\underline{y} \Rightarrow \underline{y}$ is an eigenvector of X which by condition (3) implies that it has zeros and ones and $\lambda \neq 0 \Rightarrow \lambda = 1$ which implies that all eigenvalues of X_1 are zeros and ones which implies that X_1 is idempotent which implies that X_i is idempotent for all i which proves condition (1) implies condition (4). [No kidding — these are the thought processes of the professor throughout the course.] Consider conditions (3) and (4): We have $k = \sum k_i$ and X is idempotent. We will show that (2) holds true. By Lagrange's reduction, $\exists Q_i$ which is non-singular such that

$$Q_i^T X_i Q_i = \begin{pmatrix} \pm 1 & & & & & & \\ & \pm 1 & & & & & \\ & & \pm 1 & & 0 & & \\ & & & \pm 1 & & & \\ & & 0 & & \ddots & & \\ & & & & & 0 & \\ & & & & & & 0 \end{pmatrix} = \begin{pmatrix} D_i & 0 \\ 0 & 0 \end{pmatrix}$$

where D_i is a $k_i \times k_i$ matrix. Let

$$\Gamma_i = Q_i^{-1} \Rightarrow X_i = \Gamma_i^T \begin{pmatrix} D_i & 0 \\ 0 & 0 \end{pmatrix} \Gamma_i = (\Gamma_{i1}^T, \ \Gamma_{i2}^T) \begin{pmatrix} D_i & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \Gamma_{i1} \\ \Gamma_{i2} \end{pmatrix} = \Gamma_{i1}^T D_i \Gamma_{i1}, i = 1, 2, ..., p \Rightarrow$$

$$X = \sum_{i=1}^p X_i = \sum_{i=1}^p \Gamma_{i1}^T D_i \Gamma_{i1} = \Gamma^T D \Gamma \text{ where } \Gamma = \begin{pmatrix} \Gamma_{11} \\ \Gamma_{21} \\ \vdots \\ \Gamma_{p1} \end{pmatrix}$$

$\sum k_i$ rows $\times$ n columns gives a $k \times n$ matrix by condition (4) and

$$D_{k\times k} = \begin{pmatrix} D_1 & & & \\ & D_2 & 0 & \\ & 0 & \ddots & \\ & & & D_p \end{pmatrix}$$

Also, $k = r(X) = r(\Gamma^T D\Gamma) \leq r(\Gamma) \Rightarrow r(\Gamma) = k$. Now, X is idempotent which implies X is non-negative definite and $\underline{y}^T X\underline{y} = \underline{y}^T\Gamma^T D\Gamma\underline{y} = \underline{z}^T D\underline{z} \geq 0, \forall\underline{z}$. There must be no -1's in D. Therefore, $D = I \Rightarrow X = \Gamma^T\Gamma$. Again, X is idempotent implies $X^2 = X \Rightarrow \Gamma^T\Gamma\Gamma^T\Gamma = \Gamma^T\Gamma$. Pre-multiply by Γ, and post-multiply by Γ^T to get $\overbrace{\Gamma\Gamma^T}^{k\times k}\Gamma\Gamma^T\overbrace{\Gamma\Gamma^T}^{k\times k}$. So, the rank $r(\Gamma\Gamma^T) = k$ implies the inverse exists since it is $k \times k$ and so, $\Gamma\Gamma^T = I$. But,

$$\Gamma\Gamma^T = \begin{pmatrix} \Gamma_{11} \\ \Gamma_{21} \\ \vdots \\ \Gamma_{p1} \end{pmatrix} (\Gamma_{11}, \ \ \Gamma_{21}, \ \ \cdots, \Gamma_{p1}) = \begin{pmatrix} \Gamma_{11}\Gamma_{11}^T & \Gamma_{11}\Gamma_{21}^T & \cdots \\ \vdots & \Gamma_{22}\Gamma_{22}^T & \cdots \\ \vdots & \ddots & \vdots \end{pmatrix}$$

which is a partitioned matrix with (i, j) partition $\Gamma_{i1}\Gamma_{j1}^T$. Therefore, any elements of the diagonal are zero since it is equal to I. Therefore, $\Gamma_{i1}\Gamma_{j1}^T = 0, \forall i \neq j$. Also, $X_iX_j = \Gamma_{i1}^T \overbrace{\Gamma_{i1}\Gamma_{j1}^T}^{=0} \Gamma_{j1} = 0$ implies condition (2) is proven.

Lemma 2.6: Let matrix A be symmetric and let matrix B be symmetric and non-negative definite. Then, $\underline{x}^T AB\underline{x} = 0\forall\underline{x} \Rightarrow AB = BA = 0$. **proof:** Let $k = rank(A)$. Let $\underline{\delta}_1, \underline{\delta}_2, ..., \underline{\delta}_k$ be k independent eigenvectors of A corresponding to the k non-zero eigenvalues of $\lambda_1, \lambda_2, ..., \lambda_k$. Now, $\underline{\delta}_i^T AB\underline{\delta}_i = \lambda_i\underline{\delta}_i^T B\underline{\delta}_i = 0 \Rightarrow \underline{\delta}_i^T B\underline{\delta}_i = 0 \Rightarrow B\underline{\delta}_i = \underline{0} \Rightarrow BC = 0$ where $C = (\underline{\delta}_1, \underline{\delta}_2, ..., \underline{\delta}_k)$. Now $\varrho(A) = \varrho(C)$. So, $A = CW$. Post-multiply to take LIN combinations of columns. Therefore, $BCW = 0$. But, $CW = 0$ and $BA = 0 \Rightarrow (BA)^T = A^TB^T = AB = 0$. Some other results that we will need on positive definite matrices are in Chapters 3 and 5 of the text book.

1. If matrix V is positive definite, then $\Re(X^TV^{-1}X) = \Re(X^TX) = \Re(X)$. This generalizes to a homework problem.

   Corollary: The rank $r(X^TV^{-1}X) = r(X)$.

   Corollary: If matrix X has full column rank, then $X^TV^{-1}X$ is non-singular and hence positive definite. More generally, $X^TV^{-1}X$ is non-negative definite.

2. The column space $\varrho(X(X^TV^{-1}X)^-X^T) = \varrho(X)$ if V is positive definite. This generalizes to a homework problem.

   Corollary: The rank $r(X) = r(X(X^TV^{-1}X)^-X^T)$.

15.9 Homework and Answers

1. Let A, Γ, and $\lambda_1, \lambda_2, ..., \lambda_n$ be as in Corollary 2.1, and let $\underline{\gamma}_i$ be the i^{th} row of Γ. Do the following.

   (a) Show that $A = \sum_{i=1}^n \lambda_i\underline{\gamma}_i\underline{\gamma}_i'$. We know that $\Gamma A\Gamma^T = D(\lambda_i), \exists\Gamma$ orthogonal.

$A = \Gamma^T D(\lambda_i)\Gamma =$

$$(\underline{\gamma}_1, \underline{\gamma}_2, ..., \underline{\gamma}_n) \begin{pmatrix} \lambda_1 & \cdots & \cdots & 0 \\ \vdots & \lambda_2 & \cdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & \lambda_n \end{pmatrix} \begin{pmatrix} \underline{\gamma}_1^T \\ \underline{\gamma}_2^T \\ \vdots \\ \underline{\gamma}_n^T \end{pmatrix} = (\underline{\gamma}_1, \underline{\gamma}_2, ..., \underline{\gamma}_n) \begin{pmatrix} \underline{\lambda}_1 \underline{\gamma}_1^T \\ \underline{\lambda}_2 \underline{\gamma}_2^T \\ \vdots \\ \underline{\lambda}_n \underline{\gamma}_n^T \end{pmatrix} = \sum_{i=1}^{n} \lambda_i \underline{\gamma}_i \underline{\gamma}_i^T.$$

(b) Suppose the rank $r(A) = k < n$. Show that exactly k of the λ_i's are non-zero. Multiplication by a non-singular matrix does not change rank. $\Gamma^T A \Gamma = D(\lambda_i)$, where Γ are the orthogonal vectors of matrix A. Then, $A = \Gamma D(\lambda_i)\Gamma^T$. The rank $r(A) = r(\Gamma D(\lambda_i)\Gamma^T) = k < n$.

(c) Suppose further that A is idempotent and that the rank $r(A) = k$. Write $A_i = \lambda_i \underline{\gamma}_i \underline{\gamma}_i'$. Show explicitly that the non-zero A_i's satisfy all 4 conditions of Theorem 2.2. $A_i = \lambda_i \underline{\gamma}_i \underline{\gamma}_i^T$ because $\lambda_i = 1$. There are k of these by (b).

i. $A_i^2 = \underline{\gamma}_i \underline{\gamma}_i^T \underline{\gamma}_i \underline{\gamma}_i^T = \underline{\gamma}_i \underline{\gamma}_i^T = A_i = 1$ since Γ is orthogonal.

ii. $A_i A_j = 0 = \underline{\gamma}_i \underline{\gamma}_i^T \underline{\gamma}_i \underline{\gamma}_i^T = 0$ because $\underline{\gamma}_i^T \underline{\gamma}_i = 0$.

iii. $\sum_{i=1} A_i = \sum_{i=1} \underline{\gamma}_i \underline{\gamma}_i^T = A$ given A is idempotent.

iv. $r(A) = k = \sum_{i=1}^{k} r(A_i) = \sum_{i=1}^{k} 1$. Since $r(A_i) = tr(A_i) = tr(\underline{\gamma}_i \underline{\gamma}_i^T) = tr(\underline{\gamma}_i^T \underline{\gamma}_i) = tr(1) = 1$.

2. For Theorem 2.2 give counter examples to show that:

(a) Conditions (a) and (d) do not imply all four conditions. HINT: Use 2×2 matrices.

$$x_2 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

$$x_2 x_2 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \neq x_2 \Rightarrow \text{ not idempotent.}$$

x_2 is not symmetric either.

(b) Conditions (b) and (d) do not imply all four conditions. HINT: Use 2×2 matrices. Let

$$x_1 = \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & 0 \end{pmatrix}$$

and

$$x_2 = \begin{pmatrix} 0 & 0 \\ 0 & -\frac{1}{2} \end{pmatrix}.$$

$r(x_1) + r(x_2) = 1 + 1 = 2.$

$$X = \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} \Rightarrow r(X) = 2.$$

Conditions (b) and (d) are satisfied.

$$\begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

Is X idempotent?

$$X^2 = \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix} \neq X \Rightarrow \text{ disproves (c)}$$

Is x_1 idempotent?

$$x_1^2 = \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} -\frac{1}{2} & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{4} & 0 \\ 0 & 0 \end{pmatrix} \neq x_1 \Rightarrow \text{ disproves (a)}$$

3. Prove the following.

(a) For any $A_{m\times n}$ and $B_{n\times m}$ matrices, the trace $tr(AB) = tr(BA)$.

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix}, \quad B = \begin{pmatrix} b_{11} & b_{12} & \cdots & b_{1m} \\ b_{21} & b_{22} & \cdots & b_{2m} \\ \vdots & \vdots & \cdots & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{nm} \end{pmatrix}.$$

So, $tr(AB) = \sum_{i=1}^n a_{1i}b_{i1} + \sum_{i=1}^n a_{2i}b_{i2} + \cdots + \sum_{i=1}^n a_{mi}b_{im} = \sum_{j=1}^m \sum_{i=1}^n a_{ji}b_{ij}$. And, $tr(BA) = \sum_{i=1}^m b_{1i}a_{i1} + \sum_{i=1}^m b_{2i}a_{i2} + \cdots + \sum_{i=1}^m b_{ni}a_{in} = \sum_{j=1}^n \sum_{i=1}^m b_{ji}a_{ij} = \sum_{j=1}^m \sum_{i=1}^n a_{ji}b_{ij} = tr(AB)$.

(b) If matrix A is symmetric with eigenvalues $\lambda_1, \lambda_2, ..., \lambda_n$, then $tr(A) = \sum_{i=1}^n \lambda_i$. Suppose $\Gamma A \Gamma^T = D(\lambda_i)$. Then,

$$A\Gamma^T = \Gamma^T D(\lambda_i), \quad A = \Gamma^T D(\lambda_i)\Gamma,$$

Then by Corollary 2.1,

$$tr(A) = tr(\Gamma^T D(\lambda_i)\Gamma) = tr(\Gamma\Gamma^T D(\lambda_i)) = tr(D(\lambda_i)) = \sum_{i=1}^n \lambda_i$$

by definition of the trace function. The matrices can be reordered inside the trace function according to *CRC* 27-th Edition, page 37. Dr Morgan pointed out that part (a) of this problem let's you do this also.

(c) If matrix A is symmetric and idempotent, then $tr(A) = r(A)$. Matrix A is both idempotent and symmetric. Then, we know that the λ_i's are either 0 or 1. Suppose matrix A has rank k. Then, by question (3b), $tr(A) = \sum_{i=1}^n \lambda_i = k$ from question (1b). Thus, $tr(A) = r(A) = k$.

4. Prove the following.

(a) $r(A) \geq r(BA)$. Consider the row space of each matrix. The rows of BA are linear combinations of the rows of A. Therefore, $\Re(BA) \subseteq \Re(A) \Rightarrow r(BA) \leq r(A)$ since the rank of matrix A is equal to the number of LIN rows it contains.

(b) $r(X) = r(X(X'X)^- X')$, where $G = (X'X)^-$ is a generalized inverse of $X'X$. $r(X) \geq r(X(X^TX)^- X^T)$ from (4a). $r(X(X^TX)^-X^T) \geq r(X \overbrace{(X^TX)^-X^T}^{\text{g-inverse of } X} X) = r(X) \Rightarrow r(X) = r(X(X^TX)^-)X^T)$ by Lemma 1.5.

(c) $\Re(X) = \Re(X'X)$. The reasoning is the same as in (a). $\Re(X^TX) \subseteq \Re(X)$. So, if $r(X^TX) = r(X)$, we are done. $r(X) \geq r(X^TX)$. $r(X^TX) \geq r(X^T(X^TX)^-X^TX) \Rightarrow r(X) = r(X^TX)$.

(d) Conclude that $\varrho(X) = \varrho(XX')$. Write $Y = X^T$ Then by part (c), $\Re(Y^TY) = \Re(Y) \Rightarrow \Re(XX^T) = \Re(X^T) \Rightarrow \varrho(XX^T) = \varrho(X)$ by symmetry.

5. Let the matrix A be given by

$$A = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}.$$

Note that A is idempotent and that the rank $r(A) = 2$.

(a) Find the matrices A_1 and A_2 mentioned in part (c) of problem 1. By solving $|A - \lambda I| = 0$, yields $\lambda_1 = 0, \lambda_2 = 1$, and $\lambda_3 = 1$. For $\lambda_1 = 0$,

$$\begin{pmatrix} \frac{1}{2} - 0 & 0 & \frac{1}{2} \\ 0 & 1 - 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} - 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \underline{\gamma}_1^T = \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}.$$

For $\lambda_2 = 1$ and $\lambda_3 = 1$,

$$\begin{pmatrix} -\frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \underline{\gamma}_2^T = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \ \underline{\gamma}_3^T = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

$$\Gamma^T \Gamma = \begin{pmatrix} -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 1+0+1 & -1+0+1 & 0 \\ -1+0+1 & 1+0+1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \Rightarrow$$

must multiply $\Gamma^T \Gamma$ by $\frac{1}{\sqrt{2}}$ to get the identity matrix. So, finally

$$\underline{\gamma}_1 = \begin{pmatrix} -\frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \ \underline{\gamma}_2 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}, \ \underline{\gamma}_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

Find A_2.

$$A_2 = \lambda_2 \underline{\gamma}_2 \underline{\gamma}_2^T = 1 \times \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \left(\frac{1}{\sqrt{2}}, \ 0, \ \frac{1}{\sqrt{2}} \right) = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}.$$

The problem with solving for A_1 this way is that it results in a matrix of zeros. Dr Morgan didn't like that answer.

(b) Find a third matrix A_3 so that A_1, A_2, and A_3 satisfy the conditions of Theorem 2.2. Choose A_3 so that

$$A_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Are the A_i's idempotent?

$$A_2^2 = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{4}+0+\frac{1}{4} & 0 & \frac{1}{4}+\frac{1}{4}+0 \\ 0 & 0 & 0 \\ \frac{1}{4}+0+\frac{1}{4} & 0 & \frac{1}{4}+\frac{1}{4}+0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \Rightarrow$$

matrix A_2 is idempotent. Matrices A_1 and A_3 are obviously idempotent. Does $x_i, x_j = 0, \forall(i \neq j)$? $A_1 A_j = 0, \forall j$:

$$A_2 A_3 = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

$$A_3 A_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Therefore (b) is satisfied.

$$A = A_1 + A_2 + A_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}$$

$$A^2 = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{4}+\frac{1}{4} & 0 & \frac{1}{4}+\frac{1}{4} \\ 0 & 1 & 0 \\ \frac{1}{4}+\frac{1}{4} & 0 & \frac{1}{4}+\frac{1}{4} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \Rightarrow$$

matrix A is idempotent which implies (c) is satisfied. $k = sum_{i=1}^{3} k_i = 0 + 1 + 1 = 2 = r(A) \Rightarrow$ part (d) is satisfied.

(c) What is $A_1 + A_2 + A_3$? It equals to λI perhaps.

15.10 Normal, F, t, and χ^2 Distributions

Let

$$\underline{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

be a *random vector* or a vector of random variables. Define the expected value $E(\underline{x})$ as the vector of the expected values of the variables

$$E(\underline{x}) = \begin{pmatrix} E(x_1) \\ E(x_2) \\ \vdots \\ E(x_n) \end{pmatrix} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_n \end{pmatrix} = \underline{\mu}.$$

Define $Var(\underline{x})$ as the $n \times n$ matrix whose (i, j) element is $Cov(x_i, x_j)$. It follows that $Var(\underline{x}) = E[(\underline{x} - \underline{\mu})(\underline{x} - \underline{\mu})^T]$. Note that the i-th diagonal element is $Var(x_i)$. If $\underline{x}_n$ is an $n \times 1$ vector and $\underline{y}_m$ is an $m \times 1$ vector, we define the covariance as $Cov(\underline{x}, \underline{y})$ as the $n \times m$ matrix with the (i, j) entry as $Cov(x_i, y_j)$. $Cov(\underline{x}, \underline{y}) = E[(\underline{x} - \underline{\mu}_x)(\underline{y} - \underline{\mu}_y)^T]$. Note that $Cov(\underline{x}, \underline{x}) = Var(\underline{x})$. What happens to these expressions under linear transformations? Let the matrices A and B be matrices of constants. $E(A\underline{x}) = AE(\underline{x}) = A\underline{\mu}_x$. $Cov(A\underline{x}, B\underline{y}) = E[(A\underline{x} - A\underline{\mu}_x)(B\underline{y} - B\underline{\mu}_y)^T] = E[A(\underline{x} - \underline{\mu}_x)(\underline{y} - \underline{\mu}_y)B^T] = A\,Cov(\underline{x}, \underline{y})B^T$. In particular, $Cov(A\underline{x}, B\underline{x}) = A\,Cov(\underline{x}, \underline{x})B^T = A\,Var(\underline{x})B^T$. $Var(A\underline{x}) = A\,Var(\underline{x})A^T = AVA^T$ where $V = Var(\underline{x})$. If we let A be a vector, say $A = \underline{\ell}^T_{1\times n}$, then $Var(\underline{\ell}^T\underline{x}) = \underline{\ell}^T V \underline{\ell}$ is the variance of that random vector and is greater than or equal to zero. A variance matrix must be non-negative definite. We define the moment generating function of $\underline{x}$ by

$$M_{\underline{x}}(\underline{t}) = E[e^{\underline{t}^T\underline{x}}] = \int \cdots \int e^{\underline{t}^T\underline{x}} f(\underline{x}) dx_1, ..., dx_n$$

where $f(\underline{x})$ is the density for $\underline{x}$. Recall from STAT 625 that $M_{\underline{x}}(\underline{t}) = \prod_{i=1}^n M_{x_i}(t_i)$ iff x_i are independent.

Example: Let x_1, x_2, x_3, x_4 be independent normals with common variance 1 and means 0, 1, -1, and 2. Then

$$\underline{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_2 \\ x_4 \end{pmatrix}, \; E(\underline{x}) = \begin{pmatrix} 0 \\ 1 \\ -1 \\ 2 \end{pmatrix} = \underline{\mu}, \; Var(\underline{x}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \; A^T = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 \end{pmatrix}.$$

Let $\underline{y}_{3\times 1} = A^T_{3\times 4}\underline{x}_{4\times 1}$.

$$E(\underline{y}) = A^T\underline{\mu} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 2 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ -2 \end{pmatrix}.$$

$$Var(\underline{y}) = Var(A^T\underline{x}) = A^T Var(\underline{x}) A = A^T A = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix}.$$

15.10.1 Multivariate Normal Distribution

If $z_1, z_2, ..., z_n$ are independent normals each with mean zero and variance 1, $A_{n\times n}$ is a non-singular matrix of constants and $\underline{\mu}_{n\times 1}$ is a vector of constants then, $\underline{x} = A\underline{z} + \underline{\mu}$, $\underline{z}^T = (z_1, z_2, ..., z_n)$ is a *multivariate normal.*

1. The density of $\underline{x}$ is

$$f_{\underline{z}}(\underline{z}) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}z_i^2} = \frac{1}{(2\pi)^{n/2}} \exp\Big\{ -\frac{1}{2}\underline{z}^T\underline{z}\Big\}, \; \underline{x} = A\underline{z} + \underline{\mu}, \; \underline{z} = A^{-1}(\underline{x} - \underline{\mu}) \Rightarrow$$

the Jacobian (using the determinant)

$$\frac{d\underline{z}}{d\underline{x}} = A^{-1} \Rightarrow J = |A^{-1} = |A|^{-1}.$$

$$f_{\underline{x}}(\underline{x}) = f_{\underline{z}}(A^{-1}(\underline{x} - \underline{\mu}))|A|^{-1} = \frac{1}{(2\pi)^{n/2}} \frac{1}{|A|} \exp\Big\{ -\frac{1}{2}(\underline{x} - \underline{\mu})^T (A^{-1})^T A^{-1} (\underline{x} - \underline{\mu})\Big\} =$$

$$\frac{1}{(2\pi)^{n/2}} \frac{1}{|A|} \exp\Big\{ -\frac{1}{2}(\underline{x} - \underline{\mu})^T V^{-1} (\underline{x} - \underline{\mu})\Big\}.$$

Note that $Var(\underline{x}) = Var(A\underline{z} + \underline{\mu}) = Var(A\underline{z}) = A\overbrace{Var(\underline{z})}^{=I}A^T = AA^T = V$, say. Then, also note that

$$|V| = |AA^T| = |A||A^T| = |A|^2.$$

So we obtain

$$\frac{1}{(2\pi)^{n/2}|V|^{1/2}}\exp\bigg\{-\frac{1}{2}(\underline{x}-\underline{\mu})^T V^{-1}(\underline{x}-\underline{\mu})\bigg\}.$$

Special cases occur when $n = 1$ which is the normal distribution and $n = 2$ which is the bivariate normal distribution.

2. Given matrix A had been singular, we would have arrived at the singular *singular multivariate normal distribution.* Note V^{-1} does not exist. The text book has some results for this case.

3. The case $\underline{x} \sim N(\underline{\mu}, V)$ can always be transformed to $\underline{y} \sim N(\underline{0}, I)$. Since V is positive definite, $V = H^T H$ where H is non-singular can always be obtained. Let $\underline{y} = (H^T)^{-1}(\underline{x} - \underline{\mu})$. The moment generating function is $\exp\bigg\{\underline{t}^T\underline{\mu} + \frac{1}{2}\underline{t}^T V\underline{t}\bigg\}$.

4. The marginals are multivariate normal. In particular, $A_1\underline{x}$ is multivariate normal whenever A_1 has full row rank p. **proof:** Let $p < n$. A_2 is such that the rows of A_2 are orthogonal to the rows of A_1 and $r(A_2) = n - p$. Redefine A_2. $A_2 \ni$: A_2 satisfies $A_2 V A_1^T = 0$ and $r(A_2) = n - p$. $\underline{y}_1 = A_1\underline{x}$. $\underline{y}_2 = A_2\underline{x}$. $Cov(\underline{y}_1, \underline{y}_2) = Cov(A_1\underline{x}, A_2\underline{x}) = A_1 Cov(\underline{x}, \underline{x})A_2^T = A_1 V A_2^T = (A_2 V A_1^T)^T = 0$. In fact, $\underline{y}_1$ and $\underline{y}_2$ are independent and factor into two pieces. $\underline{y}_2 \sim N(A_2\underline{\mu}, A_2 V A_2^T)$ and $\underline{y}_1 \sim N(A_1\underline{\mu}, A_1 V A_1^T)$.

15.10.2 Non-Central Chi-Square Distribution

If $\underline{x}_{n\times 1} \sim N(\underline{0}, \underline{I})$, then $\underline{x}^T\underline{x} = \sum_{i=1}^n x_i^2 \sim \chi^2(n)$. The distribution of $\underline{x}^T\underline{x}$ when $\underline{x} \sim N(\underline{\mu}, \underline{I})$ is called *non-central chi-square* and the symbol is $\chi^{2\prime}(n, \lambda)$, where n is the degrees of freedom, and $\lambda = \frac{1}{2}\underline{\mu}^T\underline{\mu} = \frac{1}{2}\sum_{i=1}^n \mu_i^2$. The density is

$$g(z) = \sum_{j=0}^{\infty}\frac{e^{-\lambda}\lambda^j}{j!}\left(\frac{1}{2}\right)^{\frac{2j+n}{2}}\frac{1}{\Gamma\left(\frac{2j+n}{2}\right)}e^{-z/2}z^{\frac{2j+n}{2}-1}, z > 0$$

which looks like a combination of both a Poisson and a chi-square distribution. The moment generating function is

$$E(e^{tz}) = \int_0^{\infty}\sum_{j=0}^{\infty}\frac{e^{-\lambda}\lambda^j}{j!}\left(\frac{1}{2}\right)^{\frac{2j+n}{2}}\frac{1}{\Gamma\left(\frac{2j+n}{2}\right)}e^{-z/2+tz}z^{\frac{2j+n}{2}-1}dz =$$

$$\sum_{j=0}^{\infty}\frac{e^{-\lambda}\lambda^j}{j!}\underbrace{\int_0^{\infty}e^{tz}\left(\frac{1}{2}\right)^{\frac{2j+n}{2}}\frac{1}{\Gamma\left(\frac{2j+n}{2}\right)}e^{-z/2}z^{\frac{2j+n}{2}-1}dz}_{\text{chi-square with } 2j+n \text{ df}} =$$

$$e^{-\lambda}(1-2t)^{-\frac{n}{2}}\sum_{j=0}^{\infty}\frac{[\lambda(1-2t)^{-1}]^j}{j!} = e^{-\lambda}(1-2t)^{-\frac{n}{2}}e^{\lambda(1-2t)^{-1}} =$$

$$(1-2t)^{-\frac{n}{2}}e^{-\lambda[1-(1-2t)^{-1}]}$$

which is a non-central chi-square moment generating function. To calculate the moments $x \sim N(\mu, \sigma) \Rightarrow E(x^2) = \mu^2 + \sigma^2$. $E(x^4) = 6\mu^2\sigma^2 + \mu^4 + 3\sigma^4$. $\sigma = 1 \Rightarrow E(x^2) = \mu^2 + 1$ and $E(x^4) = 6\mu^2 + \mu^4 + 3$. So,

$$E\left(\sum_{i=1}^{n} x_i^2\right) = \sum_{i=1}^{n} E(x_i^2) = \sum_{i=1}^{n}(1+\mu_i^2) = n + \underline{\mu}^T\underline{\mu} = n + 2\lambda.$$

To find the variance,

$$Var\left(\sum_{i=1}^{n} x_i^2\right) = \sum_{i=1}^{n} Var(x_i^2) = \sum_{i=1}^{n}[E(x_i^4) - (E(x_i^2))^2] = \sum_{i=1}^{n}\left\{[6\mu_i^2 + \mu_i^4 + 3] - [1 + 2\mu_i^2 + \mu^4]\right\} =$$

$$\sum_{i=1}^{n}(4\mu_i^2 + 2) = 4\underline{\mu}^T\underline{\mu} + 2n = 8\lambda + 2n.$$

15.10.3 Non-central F Distribution

Let $v_1 \sim \chi^2(n_1, \lambda)$ and $v_2 \sim \chi^2(n_2)$ and both v_1 and v_2 are independent. $\frac{v_1/n_1}{v_2/n_2}$ has a non-central F distribution denoted by $F'(n_1, n_2, \lambda)$ where n_1 is the numerator degrees of freedom, n_2 is the denominator degrees of freedom and λ is the non-centrality parameter. The density function of the non-central F distribution is

$$f(v|n_1, n_2, \lambda) = \sum_{k=0}^{\infty} \frac{e^{-\lambda}\lambda^k}{k!} \frac{n_1^{(\frac{1}{2}n_1 k)} n_2^{(\frac{1}{2}n_2)} \Gamma(\frac{1}{2}n_1 + \frac{1}{2}n_2 + k)}{\Gamma(\frac{1}{2}n_1 + k)\Gamma(\frac{1}{2}n_2)} \frac{v^{(\frac{1}{2}n_1 + k - 1)}}{(n_2 + n_1 v)^{(\frac{1}{2}n_1 + \frac{1}{2}n_2 + k)}}.$$

The mean is given by

$$E(v) = \frac{n_2}{n_2 - 2}\left(1 + \frac{2\lambda}{n_1}\right).$$

The variance is given by

$$Var(v) = \frac{2n_2^2}{n_1^2(n_2-2)}\left[\frac{(n_1+2\lambda)^2}{(n_2-2)(n_2-4)} + \frac{(n_1+4\lambda)}{n_2-4}\right], n_2 \geq 4.$$

15.10.4 Distributions of Quadratic Forms

Theorem 2.3: Let the random vector $\underline{x}$ have mean $\underline{\mu}$ and a variance matrix V where V is positive definite. Then,

1. $E(\underline{x}^T A\underline{x} = tr(AV) + \underline{\mu}^T A\underline{\mu}$. If also $\underline{x} \sim N(\underline{\mu}, V)$ and A is symmetric, then this implies (2).
2. $Cov(\underline{x}, \underline{x}^T A\underline{x}) = 2VA\underline{\mu}$.
3. $Var(\underline{x}^T A\underline{x}) = 2tr\left([AV]^2\right) + 4\underline{\mu}^T AVA\underline{\mu}$.

Proof:

1. $E(\underline{x}^T A\underline{x}) = E(tr(\underline{x}^T A\underline{x})) = E(A\underline{x}\underline{x}^T) = tr(AE(\underline{x}\underline{x}^T)) = tr(A[V + \underline{\mu}\underline{\mu}^T]) = tr(AV) + tr(A\underline{\mu}\underline{\mu}^T) = tr(AV) + tr(\underline{\mu}^T A\underline{\mu}) = tr(AV) + \underline{\mu}^T A\underline{\mu}$.

2. $Cov(\underline{x}, \underline{x}^T A\underline{x}) = E[(\underline{x}-\underline{\mu})(\underline{x}^T A\underline{x} - tr(AV) - \underline{\mu}^T A\underline{\mu})] = E[(\underline{x}-\underline{\mu})[(\underline{x}-\underline{\mu})^T A(\underline{x}-\underline{\mu}) + 2(\underline{x}-\underline{\mu})^T A\underline{\mu} - tr(AV)]] = \overbrace{E[(\underline{x}-\underline{\mu})^T(\underline{x}-\underline{\mu})^T A(\underline{x}-\underline{\mu})]}^{=0} + \overbrace{2E[(\underline{x}-\underline{\mu})(\underline{x}-\underline{\mu})^T A\underline{\mu}]}^{=2VA\mu \text{ variance}} - \overbrace{E[(\underline{x}-\underline{\mu}) + r(AV)]}^{=0}$

3. Write $V = HH^T$ where H is non-singular. Let $\underline{y} = H^{-1}(\underline{x}-\underline{\mu})$ i.e. $\underline{x} = H\underline{y}+\underline{\mu}$ and $\underline{y} \sim N(\underline{0}, I) \Rightarrow \underline{x}^T A\underline{x} = (H\underline{y}+\underline{\mu})^T A(H\underline{y}+\underline{\mu}) = \underline{y}^T H^T AH\underline{y} + 2\underline{\mu}^T AH\underline{y} + \underline{\mu}^T A\underline{\mu} \Rightarrow Var(\underline{x}^T A\underline{x}) = Var(\underline{y}^T \overbrace{H^T AH}^{\text{call it } B} \underline{y}) + 4Cov(\underline{y}^T H^T AH\underline{y}, \underline{\mu}^T AH\underline{y}) + 4Var(\underline{\mu}^T AH\underline{y}) = Var(\underline{y}^T B\underline{y}) + 4\underline{\mu}^T AH\overbrace{Cov(\underline{y}, \underline{y}^T B\underline{y})}^{2IB\underline{0}=\underline{0}} + 4\underline{\mu}^T AHIH^T A\underline{\mu} = Var(\underline{y}^T B\underline{y}) + 4\underline{\mu}^T AVA\underline{\mu} = Var(\underline{x}^T A\underline{x})$. So, $Var(\underline{y}^T B\underline{y}) = E([\underline{y}^T B\underline{y}]^2) - (E(\underline{y}^T B\underline{y}))^2 = E([\underline{y}^T B\underline{y}]^2) - [tr(BI)+\underline{0}]^2 = E([\underline{y}^T B\underline{y}]^2) - (tr(B))^2$. So, $(\underline{y}^T B\underline{y})^2 = \underline{y}^T B\underline{y}\underline{y}^T B\underline{y} = tr(\underline{y}^T B\underline{y}\underline{y}^T B\underline{y}) = tr(B\underline{y}\underline{y}^T B\underline{y}\underline{y}^T) = tr(B\underline{y}\underline{y}^T\underline{y}^T B\underline{y})$. Therefore, $E(\underline{y}^T B\underline{y})^2 = E\left\{tr(B\underline{y}\underline{y}^T\underline{y}^T B\underline{y})\right\} = tr(B\ E(\overbrace{\underline{y}\underline{y}^T}^{n\times n}\ \overbrace{\underline{y}^T B\underline{y}}^{\text{scalar}}))$. Consider the elements of $\underline{y}\underline{y}^T\underline{y}^T B\underline{y}$. The diagonal element (m,m), $\underline{y}\underline{y}^T = b_{mm}y_m^2[\sum_{i=1}^n\sum_{j=1}^n y_i y_j b_{ij}] = b_{mm}y_m^4 + \sum_{j\neq m} y_m^3 y_j b_{mj} + \sum_{i\neq m} y_m^3 y_i b_{im} + \sum_{i\neq m}\sum_{j\neq m} y_m^2 y_i y_j b_{ij} \Rightarrow E((m,m)\text{ element}) = 3b_{mm} + 0 + 0 + 0 = 3b_{mm}$ because $E(x^4)$ of a $N(0,1)$ is 3. For the off-diagonal element (l,m), $y_l y_m\left[\sum_{i=1}^n\sum_{j=1}^n y_i y_j b_{ij}\right]$. The expected value of the (l,m) element is $E\left(y_l^2 y_m^2(b_{lm}+b_{ml})\right) = b_{lm} + b_{ml} = 2b_{lm}$ (since B is symmetric). Therefore, go back to the diagonal element, $\sum_{i\neq m} E(y_m^2 y_i^2)b_{ii} + b_m E(y_m^4) = 3b_{mm} + \sum_{i\neq m} b_{ii} = 2b_{mm} + \sum_{i=1}^m b_{ii} = 2b_{mm} + tr(B) \Rightarrow E(\underline{y}\underline{y}^T\underline{y}^T B\underline{y}) = 2B + [tr(B)]I \Rightarrow E(\underline{y}^T B\underline{y})^2 = tr\left\{B[2B + tr(B)I\right\} = tr\left\{2B^2\right\} + [tr(B)]^2 \Rightarrow Var(\underline{y}^T B\underline{y}) = 2tr\left\{B^2\right\} = 2tr\left\{H^T AHH^T AH\right\} = 2tr\left\{AHH^T AHH^T\right\} = 2tr\left\{AVAV\right\}$. This matches the other part of the theorem.

Lemma 2.7: Assume that $\underline{x} \sim N(\underline{\mu}, I)$ and the matrix A is symmetric. The mgf of $\underline{x}^T A\underline{x}$ is

$$M_{\underline{x}^T A\underline{x}} = \exp\left\{-\frac{1}{2}\underline{\mu}^T\left[I - (I-2tAV)^{-1}\right]V^{-1}\underline{\mu}\right\}|I-2tAV|^{-\frac{1}{2}}$$

proof:

$$M_{\underline{x}^T A\underline{x}} = \frac{1}{(2\pi)^{\frac{n}{2}}|V|^{\frac{1}{2}}}\int\cdots\int \exp\left\{t\underline{x}^T A\underline{x}\right\}\exp\left\{-\frac{1}{2}(\underline{x}-\underline{\mu})^T V^{-1}(\underline{x}-\underline{\mu})\right\}dx_1 dx_2\cdots dx_n =$$

$$\int\cdots\int \overbrace{\frac{\exp\left\{-\frac{1}{2}\underline{\mu}^T V^{-1}\underline{\mu}\right\}}{(2\pi)^{\frac{n}{2}}|V|^{\frac{1}{2}}}}^{\text{a constant } c}\exp\left\{-\frac{1}{2}\underline{x}^T V^{-1}\underline{x} + t\underline{x}^T A\underline{x} + \underline{\mu}^T V^{-1}\underline{x}\right\} =$$

$$c\int\cdots\int \exp\left\{-\frac{1}{2}\underline{x}^T V^{-1}(V-2tVAV)V^{-1}\underline{x} + \underline{\mu}^T V^{-1}\underline{x}\right\}\prod_{i=1}^n dx_i.$$

Let $y = V^{-1}\underline{x} \Rightarrow x = Vy \Rightarrow J = \left|\frac{dx}{dy}\right| = |V|$. Then,

$$c_1\int\cdots\int \exp\left\{-\frac{1}{2}\underline{y}^T W\underline{y} + \underline{\mu}^T\underline{y}\right\}\prod_{i=1}^n dx_i$$

where $c_1 = |V|c$ and $W = V - 2tVAV$. Then,

$$c_1\int\cdots\int \exp\left\{-\frac{1}{2}(\underline{y} - \overbrace{W^{-1}\underline{\mu}}^{\text{mean}})^T\overbrace{W}^{\text{covar}}(\underline{y} - W^{-1}\underline{\mu}) + \frac{1}{2}\underline{\mu}^T W\underline{\mu}\right\}\prod_{i=1}^n dy_i =$$

$$c_1 \exp\left\{\frac{1}{2}\underline{\mu}^T W\underline{\mu}\right\}(2\pi)^{\frac{n}{2}}|W|^{-\frac{1}{2}} = \exp\{-\frac{1}{2}[\underline{\mu}^T(V^{-1}-W^{-1})\underline{\mu}]\}|V|^{\frac{1}{2}}|W|^{-\frac{1}{2}} =$$

$$\exp\left\{-\frac{1}{2}\left[\underline{\mu}^T(V^{-1}-(V-2tVAV)^{-1})\underline{\mu}\right]\right\}|V|^{\frac{1}{2}}|V-2tVAV|^{-\frac{1}{2}} =$$

$$\exp\left\{-\frac{1}{2}\left[\underline{\mu}^T(I-(I-2tAV)^{-1})V^{-1}\underline{\mu}\right]\right\}|I-2tAV|^{-\frac{1}{2}}.$$

Theorem 2.4: Let $\underline{x} \sim N(\underline{\mu}, V)$ and the matrix A is symmetric. Then, $\underline{x}^T A\underline{x} \sim \chi^2\left(r(A), \frac{1}{2}\underline{\mu}^T A\underline{\mu}\right) \Leftrightarrow AV$ is idempotent. proof: From Lemma 2.7, the mgf of $\underline{x}^T A\underline{x}$ is

$$|I-2tAV|^{-\frac{1}{2}}\exp\left\{-\frac{1}{2}\underline{\mu}^T\left[I-(I-2tAV)^{-1}\right]V^{-1}\underline{\mu}\right\} =$$

$$\prod_{i=1}^{n}(1-2t\lambda_i(AV))^{-\frac{1}{2}}\exp\left\{-\frac{1}{2}\underline{\mu}^T\left[I-(I-2tAV)^{-1}\right]V^{-1}\underline{\mu}\right\}$$

where λ_i are eigenvalues of AV.

1. Suppose that AV is idempotent. Then, $I-(I-2tAV)^{-1} = [1-(1-2t)^{-1}]AV$. So, the mgf of $\underline{x}^T A\underline{x}$ is

$$\left[\prod_{i=1}^{r}(1-2t)^{-\frac{1}{2}}\right]\exp\left\{-\frac{1}{2}\underline{\mu}^T[1-(1-2t)^{-1}]A\underline{\mu}\right\} =$$

$$(1-2t)^{-\frac{r}{2}}\exp\left\{-\frac{1}{2}\underline{\mu}^T A\underline{\mu}[1-(1-2t)^{-1}]\right\}$$

which is the mgf of a $\chi^2\left(r, \frac{1}{2}\underline{\mu}^T AV\right) \Rightarrow \underline{x}^T A\underline{x}$ has this distribution.

2. Suppose that $\underline{x}^T A\underline{x} \sim \chi^2\left(r(A), \frac{1}{2}\underline{\mu}^T A\underline{\mu}\right)$ which at $\underline{\mu} = \underline{0}$ gives

$$(1-2t)^{-\frac{r}{2}} = \prod_{i=1}^{n}[1-2t\lambda_i(AV)]^{-\frac{1}{2}}, \forall t.$$

Let $u = 2t$ and raise to -2 power. Then we have,

$$(1-u)^r = \prod_{i=1}^{n}[1-u\lambda_i(AV)], \forall u \Rightarrow$$

$$(1-u)^r = \prod_{i=1}^{r}[1-u\lambda_i(AV)]$$

because of the polynomial theorem. Therefore, $\lambda_i(AV) = 1$ for $i = 1, 2, ..., r$ and $\lambda_i(AV) = 0$ for $n-r$ values of i. Note that the theorem of polynomials states that polynomials equal on an open interval must be identical.

Theorem 2.5: Assume that $\underline{x} \sim N(\underline{\mu}, V)$ and the matrix A is symmetric and non-negative definite. Then, $\underline{x}^T A\underline{x}$ and $B\underline{x}$ are independent iff $BVA = 0$. proof: Suppose that $\underline{x}^T A\underline{x}$ and $B\underline{x}$ are independent. Then, using the last part of Theorem 2.3, $\underline{0} = Cov(B\underline{x}, \underline{x}^T A\underline{x}) = BCov(\underline{x}, \underline{x}^T A\underline{x}) = 2BVA\underline{\mu}, \forall\underline{\mu} \Rightarrow BVA = \underline{0}$. Then by the definition of non-negative definite, $A = L^T L$ where $L : r(A) \times n$ and $r(L) = r(A)$. Assume that $BVA = 0$. Then, $BVA = 0 \Rightarrow BVL^T L = 0 \Rightarrow BVAL^T LL^T = 0L^T \Rightarrow BVAL^T LL^T = 0 \Rightarrow BVAL^T(LL^T)(LL^T)^{-1} = 0(LL^T)^{-1} = BVAL^T = 0$ because $r(A) \times r(A) = r(L) \times r(L)$. Therefore, $Cov(B\underline{x}, L\underline{x}) = 0 \Rightarrow B\underline{x}$ and $L\underline{x}$ are independent. Therefore, $B\underline{x}$ and $\underline{x}^T L^T L\underline{x}$ are independent. This last statement must be proven for homework. A common use of the theorem is when we have $B\underline{x}$ as an estimator and $\underline{x}^T A\underline{x}$ as an estimate of the variance of $B\underline{x}$ and we want the estimate $B\underline{x}$ to be independent of its estimated variance.

Theorem 2.6: Assume that $\underline{x} \sim N(\underline{\mu}, V)$. Assume the Matrices A and B are each non-negative definite and symmetric. Then, $\underline{x}^T A\underline{x}$ and $\underline{x}^T B\underline{x}$ are independent implies $AVB = 0$. proof: $A = L^T L, B = M^T M$ because $r(B) \times n$ and $r(M) = r(B)$. Assume that $AVB = 0$. Then, $AVB = 0 \Rightarrow BVA = 0 \Rightarrow M^T MVA = 0VA \Rightarrow MM^T MVA = M0 = (MM^T)^{-1} MM^T MVA = (MM^T)^{-1} 0 = MVA = 0$. Using Theorem 2.5, we know that $M\underline{x}$ and $\underline{x}^T A\underline{x}$ are independent. Therefore, $\underline{x}^T M^T M\underline{x}$ and $\underline{x}^T A\underline{x}$ are independent where $B = M^T M$. This implies we can assume that $\underline{x}^T A\underline{x}$ and $\underline{x}^T B\underline{x}$ are independent. The implications are that (using part of Theorem 2.3) $Var(\underline{x}^T A\underline{x} + \underline{x}^T B\underline{x}) = Var(\underline{x}^T A\underline{x}) + Var(\underline{x}^T B\underline{x}) \Rightarrow 2tr((A+B)^2 V) + 4\underline{\mu}^T(A+B)V(A+B)\underline{\mu} = 2tr(AV)^2 + 4\underline{\mu}^T A\underline{\mu} + 4tr(BV)^2 + 4\underline{\mu}^T BVB\underline{\mu}$. Now, $((A+B)V)^2 = (AV)^2 + (BV)^2 + AVBV + BVAV \Rightarrow 2tr(AVBV) + 2tr(BVAV) + 4\underline{\mu}^T AVB\underline{\mu} + 4\underline{\mu}^T BVA\underline{\mu} = 0 \Rightarrow 4tr(AVBV) + 8\underline{\mu}^T AVB\underline{\mu} = 0, \forall\underline{\mu} \Rightarrow 4tr(AVBV) = 0$ (take $\underline{\mu} = 0$) $\Rightarrow \underline{\mu}^T AVB\underline{\mu} = 0, \forall\underline{\mu}$. By Lemma 2.6, the transpose $AVB = 0 \Rightarrow BVA = 0$. An important use occurs when each quadratic form will be a sum of squares in an ANOVA table and we want them to be independent.

Theorem 2.7: Assume that $\underline{x} \sim N(\underline{\mu}, V)$. The Matrices A_i are such that they are $n \times n$ and have rank $k_i, i = 1, ..., p$. Matrix $A = \sum_{i=1}^p A_i$ has rank k. Then, $\underline{x}^T A_i\underline{x} \sim \chi^{2'}\left(k_i, \frac{1}{2}\underline{\mu}^T A_i\underline{\mu}\right)$ and $\underline{x}^T A_i\underline{x}$ are pairwise independent $i = 1, ..., p$. $\underline{x}^T A\underline{x} \sim \chi^{2'}\left(k, \frac{1}{2}\underline{\mu}^T A\underline{\mu}\right)$ and $k = \sum_{i=1}^p k_i$ iff (1) and (2) are true *or* (1) and (3) are true *or* (2) and (3) are true *or* (3) and (4) are true.

1. $A_i V$ is idempotent for $i = 1, ..., p$.
2. $A_i V A_j = 0, \forall i \neq j$.
3. AV is idempotent.
4. $k = \sum_{i=1}^p k_i$.

proof: (Uses Theorem 2.2 in the proof) $\underline{x}^T A_i\underline{x} \sim \chi^{2'}\left(k_i, \frac{1}{2}\underline{\mu}^T A_i\underline{\mu}\right)$ iff (Theorem 2.4) $A_i V$ is idempotent iff (1). $\underline{x}^T A_i\underline{x}$ and $\underline{x}^T A_j\underline{x}$ are independent iff (Theorem 2.6) $A_i V A_j = 0$ iff (2), $\underline{x}^T A\underline{x} \sim \chi^{2'}\left(k, \frac{1}{2}\underline{\mu}^T A\underline{\mu}\right)$ iff (Theorem 2.4) AV is idempotent iff (3) $\sum_{i=1}^p k_i = k$ iff (4). So, if the distributional statements are correct, then (1)-(4) are correct and hence so too are the stated pairs. Conversely, if we can show that any one of the stated pairs is correct, this implies that (1)-(4) are correct; then from what we have just written, the distributional statements will also be correct.

1. $A_i V$ idempotent implies $A_i H^T H$ is idempotent implies $A_i H^T H A_i H^T H = A_i H^T H \Leftrightarrow H A_i H^T H A_i H^T = H A_i H^T \Leftrightarrow H A_i H^T$ is idempotent.
2. $A_i V A_j = 0 \Leftrightarrow A_i H^T H A_j = 0 \Leftrightarrow H A_i H^T H A_j H^T = 0$.
3. AV is idempotent implies HAH^T is idempotent .... same for $A_i V$.

In Theorem 2.2, take $x_i = H A_i H^T$ and $x = \sum_{i=1}^p x_i = HAH^T$. This completes the proof and the end of Chapter 2 of the text book.

15.11 Homework and Answers

1. The random vector $\underline{x}$ has a $N(\underline{\mu}, V)$ distribution. Prove the following.

   (a) If $V = HH'$ for non-singular H, then $\underline{y} = H^{-1}(\underline{x} - \underline{\mu})$ has a $N(\underline{0}, I)$ distribution.

$$f_{\underline{x}}(\underline{x}) = \frac{1}{(2\pi)^{n/2}} \frac{1}{|H|} \exp\left\{-\frac{1}{2}(\underline{x} - \underline{\mu})^T (H^{-1})(H^T)^{-1}(\underline{x} - \underline{\mu})\right\} =$$

$$\frac{1}{(2\pi)^{n/2}} \frac{1}{|H|} \exp\left\{-\frac{1}{2}(\underline{x} - \underline{\mu})^T (HH^T)^{-1}(\underline{x} - \underline{\mu})\right\}.$$

   Substitute $\underline{x} = H\underline{y} + \underline{\mu}$. $\frac{dx}{d\underline{y}} = H \Rightarrow J = |H|$.

$$\frac{1}{(2\pi)^{n/2}} \frac{J}{|H|} \exp\left\{-\frac{1}{2}(H\underline{y} + \underline{\mu} - \underline{\mu})^T (HH^T)^{-1}(H\underline{y} + \underline{\mu} - \underline{\mu})\right\} =$$

$$\frac{1}{(2\pi)^{n/2}} \exp\left\{-\frac{1}{2}(H\underline{y})^T (HH^T)^{-1}(H\underline{y})\right\} =$$

$$\frac{1}{(2\pi)^{n/2}} \exp\left\{-\frac{1}{2}(H\underline{y})^T (H^T)^{-1}\underline{y}\right\} =$$

$$\frac{1}{(2\pi)^{n/2}} \exp\left\{-\frac{1}{2}\underline{y}^T H^{-1}(H\underline{y})\right\} =$$

$$\frac{1}{(2\pi)^{n/2}} \exp\left\{-\frac{1}{2}\underline{y}^T \underline{y}\right\} \sim N(\underline{0}, I).$$

   Therefore, $V = I$ and $\underline{\mu} = \underline{0}$.

   (b) For any symmetric matrix A, $E(\underline{x} - \underline{\mu})(\underline{x} - \underline{\mu})' A(\underline{x} - \underline{\mu}) = \underline{0}$. This completes the proof of Theorem 2.3 (ii). Let $\underline{y} = H^{-1}(\underline{x} - \underline{\mu})$, and $V = HH^T$. Then, $\underline{y} \sim N(\underline{0}, I)$. Find $E(H\underline{y}\underline{y}^T \overbrace{H^T A H}^{=B} \underline{y}) = HE(\underline{y}\underline{y}^T B\underline{y})$. $\underline{y}^T B\underline{y} = \sum_{i=1}^n \sum_{j=1}^n y_i y_j b_{ij}$. So, the l^{th} element of $\underline{y}\underline{y}^T\ B\underline{y}$ is $\underline{y}_l \left[\sum_{i=1}^n \sum_{j=1}^n y_i y_j b_{ij}\right] = y_l^B b_{ll} + \sum_{j=1, j\neq l}^n b_{lj} y_l^2 y_j + \sum_{i=1, i\neq l} b_{il} y_l^2 y_i + \sum_{\text{neighther } l} \sum b_{ij} y_l y_i y_j$. The expected value is $0 + 0 + 0 + 0 = 0 \Rightarrow H\underline{0} = \underline{0}$.

2. The random vector $\underline{x}$ has a $N(\underline{\mu}, V)$ distribution. Prove that the individual x_i's are independent if and only if they are uncorrelated. The correlation matrix R, is

$$R = \left\{\frac{\sigma_{ij}}{\sigma_i \sigma_j}\right\} = 0, \forall i \neq j \Rightarrow V_{ij} = 0, \forall i \neq j.$$

   Assume that the x_i's are uncorrelated. Then, $\sigma_{ij} = 0, \forall i \neq j$. Then, the mgf of $\underline{x}$ can be written as

$$\exp\left\{t_1\mu_1 + \frac{1}{2}t_1^2\sigma_{11}^2\right\} \exp\left\{t_2\mu_2 + \frac{1}{2}t_2^2\sigma_{22}^2\right\} \cdots \exp\left\{t_n\mu_n + \frac{1}{2}t_n^2\sigma_{nn}^2\right\}$$

   which implies the x_i's are independent.

3. The random vector $\underline{x}_{5\times 1}$ has a $N(\underline{\mu}, I_5)$ distribution. The matrix A is

$$A = \begin{pmatrix} \frac{2}{3} & 0 & -\frac{1}{3} & 0 & -\frac{1}{3} \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{3} & 0 & \frac{2}{3} & 0 & -\frac{1}{3} \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{3} & 0 & -\frac{1}{3} & 0 & \frac{2}{3} \end{pmatrix}$$

(a) Find the matrix B of the largest possible rank so that $\underline{x}'A\underline{x}$ and $\underline{x}'B\underline{x}$ are independent, and $\underline{x}'B\underline{x}$ has a chi-square distribution. Row reduce the matrix A.

$$\begin{pmatrix} \frac{2}{3} & 0 & -\frac{1}{3} & 0 & -\frac{1}{3} \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{3} & 0 & \frac{2}{3} & 0 & -\frac{1}{3} \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{3} & 0 & -\frac{1}{3} & 0 & \frac{2}{3} \end{pmatrix} \to \begin{pmatrix} \frac{2}{3} & 0 & -\frac{1}{3} & 0 & -\frac{1}{3} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 \end{pmatrix} \to$$

$$\begin{pmatrix} \frac{2}{3} & 0 & -\frac{1}{3} & 0 & -\frac{1}{3} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \to \begin{pmatrix} 2 & 0 & -1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \to \begin{pmatrix} 2 & 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

For the zero eigenvalues,

$$\underline{\gamma}_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}, \ \underline{\gamma}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \ \underline{\gamma}_3 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}.$$

Ignore the non-zero eigenvalues. Facts: Matrix A is symmetric. Matrix A is idempotent. AV is idempotent. The rank $r(A) = 2$. Find matrix B such that $AVB = AIB = 0$ using Theorem 2.6. $AB = 0$ implies using the orthogonal vectors found earlier. Choose

$$B = \frac{1}{3}\underline{\gamma}_1\underline{\gamma}_1^T + \underline{\gamma}_2\underline{\gamma}_2^T + \underline{\gamma}_3\underline{\gamma}_3^T = \begin{pmatrix} \frac{1}{3} & 0 & \frac{1}{3} & 0 & \frac{1}{3} \\ 0 & 1 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & 0 & \frac{1}{3} \\ 0 & 0 & 0 & 1 & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & 0 & \frac{1}{3} \end{pmatrix}.$$

Then, $B^2 = B$ and $\underline{x}^T A\underline{x}$ and $\underline{x}^T B\underline{x}$ are independent. The distribution of $\underline{x}B\underline{x}$ is chi-square.

(b) Find the matrix C of full row rank with largest possible rank so that $\underline{x}'A\underline{x}$ and $C\underline{x}$ are independent. Since the rows of C are orthogonal to the columns of A, and since the rank $r(A) = 2$, the largest possible rank of C is $5 - 2 = 3$. Hence, find matrix C which is 3×5 of rank 3 with $CA = 0$.

$$C = \begin{pmatrix} 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

(c) For the matrices A B and C above, find the distributions of $\underline{x}'A\underline{x}$, $\underline{x}'B\underline{x}$, $C\underline{x}$, and $\underline{x}'(A + B)\underline{x}$ when

i. $\underline{\mu} = \underline{0}$.

ii. $\underline{\mu} = (1, 0, 1, 0, 1)'$.
iii. $\underline{\mu} = (1, 1, 1, 1, 1)'$.

$\underline{x}^T A \underline{x} \sim \chi^2\left[2, \frac{1}{2}\underline{\mu}^T A \underline{\mu}\right]$. $\underline{x}^T B \underline{x} \sim \chi^2\left[3, \frac{1}{2}\underline{\mu}^T B \underline{\mu}\right]$. $\underline{x}^T (A+B) \underline{x} \sim \chi^2\left[5, \frac{1}{2}\underline{\mu}^T A \underline{\mu} + \frac{1}{2}\underline{\mu}^T B \underline{\mu}\right]$. $C\underline{x} \sim N(C\underline{\mu}, I)$. Note the change in λ formula for Theorem 2.7.

4. Do the following.

(a) Let $\underline{z}_{n\times 1}$ be any vector. Show that

$$\underline{z}'\left(I - \frac{1}{n}J\right)\underline{z} = \sum_{i=1}^{n}(z_i - \bar{z})^2$$

where J is an $n \times n$ matrix of $1'$s and $\bar{z} = \sum_{i=1}^{n} z_i/n$.

$$\underline{z}'\left(I - \frac{1}{n}J\right)\underline{z} = \underline{z}^T\underline{z} - \frac{1}{n}\underline{z}^T J \underline{z} = \sum_{i=1}^{n} z_i^2 - \frac{1}{n}\underline{z}^T \underline{1}\underline{1}^T \underline{z} =$$

$$\sum_{i=1}^{n} z_i^2 - \frac{1}{n}\sum_{i=1}^{n} z_i \sum_{i=1}^{n} z_i = \sum_{i=1}^{n} z_i^2 - \frac{1}{n}\left(\sum_{i=1}^{n} z_i\right)^2 = \sum_{i=1}^{n}(z_i - \bar{z})^2.$$

(b) If the random vector $\underline{x}$ has a $N(\underline{\mu}, I)$ distribution, use Theorem 2.5 to show that $\bar{x}$ and $\sum_{i=1}^{n}(x_i - \bar{x})^2$ are independent. Let $A = I - \frac{1}{n}1_{n\times n}$ and $B = \frac{1^T}{n}$. If $BVA = BA = 0$, then this would prove independence.

$$BVA = BA = \left(\frac{1}{n}, \frac{1}{n}, ..., \frac{1}{n}\right)\begin{pmatrix} \frac{n-1}{n} & -\frac{1}{n} & -\frac{1}{n} & \cdots & -\frac{1}{n} \\ -\frac{1}{n} & \frac{n-1}{n} & -\frac{1}{n} & \cdots & -\frac{1}{n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -\frac{1}{n} & -\frac{1}{n} & -\frac{1}{n} & \cdots & \frac{n-1}{n} \end{pmatrix}$$

$$\left(\frac{n-1}{n^2} - \frac{1}{n^2} - \cdots - \frac{1}{n^2}, -\frac{1}{n^2} + \frac{n-1}{n^2} - \cdots - \frac{1}{n^2}, \cdots, -\frac{1}{n^2} - \frac{1}{n^2} - \cdots + \frac{n-1}{n^2}\right) =$$

$$\frac{1}{n^2}\left((n-1)\overbrace{-1 - 1 - \cdots - 1}^{n-1 \text{ of these}}\right) = 0$$

Similar results hold for the other elements. By Theorem 2.5, $\bar{x}$ and $\sum_{i=1}^{n}(x_i - \bar{x})^2$ are independent.

(c) If the random vector $\underline{x}$ has a $N(\underline{\mu}, \sigma^2 I)$ distribution, use Theorem 2.7 to show that $(\bar{x})^2$ and $(n-1)s^2/\sigma^2$ are independent and find their distributions. Also, give the distribution of their sum. Here, $s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$. Under what condition does $(n-1)s^2/\sigma^2$ have a central chi-square distribution?

$$\frac{(n-1)s^2}{\sigma^2} = \frac{\underline{x}^T\left(I - \frac{1}{n}J\right)\underline{x}}{\sigma^2}$$

where $A_1 = \frac{(I - \frac{1}{n}J)}{\sigma^2}$. $A_1 V = (I - \frac{1}{n}J)$ which is idempotent. Therefore,

$$\frac{(n-1)s^2}{\sigma^2} \sim \chi^{2'}\left[n-1, \frac{1}{2\sigma^2}\sum_{i=1}^{n}(\mu_i-\bar{\mu})^2\right].$$

It is a central chi-square distribution iff $\mu_1 = \mu_2 = \cdots = \mu_n$. $\bar{x} = \frac{1}{n}(1\ 1\ 1\ 1\cdots 1)\underline{x} \Rightarrow (\bar{x})^2 = \underline{x}^T\frac{1}{n}\begin{pmatrix}1\\1\\\vdots\\1\end{pmatrix}\frac{1}{n}(1\ 1\ 1\ 1\cdots 1)\underline{x} = \underline{x}^T\frac{1}{n^2}J\underline{x} = \frac{\sigma^2}{n}\underline{x}^T\overbrace{\frac{1}{n\sigma^2}J}^{=A_2}\underline{x}$. $A_2V = \frac{1}{n}J$ which is idempotent. Therefore, $\underline{x}^TA_2\underline{x} \sim \chi^2\left[1, \frac{1}{2}\underline{\mu}^TA\underline{\mu}\right]$. Therefore, $(\bar{x})^2 = \frac{\sigma^2}{n}\underline{x}^TA_2\underline{x} \sim \frac{\sigma^2}{n}\chi^2\left[1, \frac{1}{2n\sigma^2}\left(\sum_{i=1}^n\mu_i\right)^2\right]$.

15.12 Test and Answers

Everyone must work problems 1 and 2. Then work two problems from among 3, 4, and 5. Work carefully and use your time wisely.

1. State completely the theorem which gives necessary and sufficient conditions for the p quadratic forms $\underline{x}'A_i\underline{x}$, $i = 1, 2, ..., p$, to have independent chi-square distributions, and for their sum to have a chi-square distribution. This is Theorem 2.7 from your class notes.

2. Consider the matrix A given by

$$A = \begin{pmatrix} 3 & 1 & -1 \\ 1 & 1 & 1 \\ -1 & 1 & 3 \end{pmatrix}$$

(a) Find a generalized inverse of matrix A. In A, column 2 is equal to $\frac{1}{2}(C_1 + C_3)$, and the upper 2×2 is non-singular. So, $r(A) = 2$. A g-inverse can be found by inverting the upper 2×2

$$\begin{pmatrix} 3 & 1 \\ 1 & 1 \end{pmatrix}^{-1} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 3 \end{pmatrix}.$$

$$G = \frac{1}{2}\begin{pmatrix} 1 & -1 & 0 \\ -1 & 3 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

(b) Use your answer in (a) to find all solutions to the equations $A\underline{x} = \underline{y}$, and then find a full set of linearly independent solutions. Here, $\underline{y} = (2, 1, 0)'$. All solutions are $G\underline{y} + (H - I)\underline{z}$ for $\underline{z} \in \Re^3$. The number of linearly independent solutions is $q - r + 1$ which is equal to the number of columns in A minus the rank $r(A) + 1 = 3 - 2 + 1 = 2$.

$$H = GA = \frac{1}{2}\begin{pmatrix} 1 & -1 & 0 \\ -1 & 3 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 3 & 1 & -1 \\ 1 & 1 & 1 \\ -1 & 1 & 3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & 2 \\ 0 & 0 & 0 \end{pmatrix}.$$

$$G\underline{y} = \frac{1}{2}\begin{pmatrix} 1 & -1 & 0 \\ -1 & 3 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} 2 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix} \text{ is one solution.}$$

$$G\underline{y} + (H-I)\underline{z} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix} + z_1 \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} + z_2 \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} + z_3 \begin{pmatrix} -1 \\ 2 \\ -1 \end{pmatrix} = \overbrace{\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix} + z_3 \begin{pmatrix} -1 \\ 2 \\ -1 \end{pmatrix}}^{\text{all solutions}}.$$

$z_3 = 0, 1 \Rightarrow 2$ independent solutions. $\left(\frac{1}{2}, \frac{1}{2}, 0\right)^T$ and $\left(-\frac{1}{2}, \frac{5}{2}, -1\right)^T$.

(c) Write down one vector $\underline{k}$ such that $\underline{k}'\underline{x}$ is invariant to the choice of solution $\underline{x}$. No proof required. Any row of H or A, e.g. $\underline{k}^T = (3,\ 1,\ -1)$.

3. X is an $m \times n$ matrix.

(a) Define what is meant by "the column space of X." $\varrho(X)$ is equal to the vector space generated by the columns of X equal to $\{X\underline{\ell} \ni: \underline{\ell} \in \Re^n\}$.

(b) Write down the expression for the matrix P_X which projects onto the column space of X. Prove it is idempotent. $P_X = X(X^TX)^-X^T$. $P_XP_X = X\overbrace{(X^TX)^-X^T}^{\text{Lem 1.5}}X(X^TX)^-X^T = X(X^TX)^-X^T \Rightarrow X(X^TX)^-X^TX = X$. Lemma 1.5 says this is a g-inverse of X.

(c) Let $Y = XM$ where M is an $n \times n$ non-singular matrix. If G is a generalized inverse of X, find an expression for a generalized inverse of Y, proving that it is a generalized inverse. Let $G_Y = M^{-1}G$. The G_Y is a g-inverse of Y, since $YG_YY = XMM^{-1}GXM = XGXM = XM = Y$.

(d) Continuing with the matrix Y as defined in (c), suppose that G_1 is a generalized inverse of $X'X$. Find an expression for a generalized inverse for $Y'Y$, and show that it is a generalized inverse. Let $G_{Y_1} = (M^{-1})G_1(M^{-1})^T$. Then, G_{Y_1} is a g-inverse of Y^TY, since $Y^TYG_{Y_1}Y^TY = (M^TX^TXM)(M^{-1})G_1(M^{-1})^T(M^TX^TXM) = M^TX^TXG_1X^TXM = M^TX^TXM = Y^TY$.

(e) Now prove that X and Y have the same column space, just by showing that the matrix P_Y that projects onto the column space of Y is identical to the one given in (b) which projects onto the column space of X. $P_Y = Y(Y^TY)^-Y^T = YG_{Y_1}Y^T = XMM^{-1}G_1(M^{-1})^TM^TX^T = XG_1X^T = P_X$.

(f) Suppose the requirement that M be non-singular is relaxed to $r(M) = r(X)$. Here matrix M is still $n \times n$. Is it now necessarily true that X and Y have the same column space? Prove or give a counter example. It is not necessarily true. Let $X = A$ of Problem 2. So, $r(X) = 2$. Let M

$$M = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 2 & 0 \\ 0 & -1 & 0 \end{pmatrix}, \quad Y = XM = \begin{pmatrix} 3 & 0 & 0 \\ 1 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}.$$

$r(M) = 2$, $r(Y) = 1 < r(X) \Rightarrow \varrho(Y) \neq \varrho(X)$.

4. A is a symmetric $n \times n$ matrix of rank k. In class, we proved the existence of an orthogonal matrix Γ such that $\Gamma A \Gamma'$ is a diagonal matrix with diagonal entries equal to the eigenvalues $\lambda_1, \lambda_2, ..., \lambda_n$ of A. Let $\underline{\gamma}_i'$ be the i^{th} row of Γ.

(a) Prove that $A = \sum_{i=1}^k \lambda_i \underline{\gamma}_i \underline{\gamma}_i'$. This was a homework problem. See page 1018 for the proof.

(b) If $k = n$ and $\lambda_1 = \lambda_2 = \cdots = \lambda_n = 1$, show that $A = I$. Can you say that the only symmetric, idempotent matrix of full rank is I? Explain. $\lambda_1 = \lambda_2 = \cdots = \lambda_n = 1 \Rightarrow \Gamma A \Gamma^T = I \Rightarrow A = \Gamma^T\Gamma = I$. Yes, since the symmetric idempotent matrices are exactly those for which all non-zero eigenvalues are 1, and to be of rank n the condition is $\lambda_1 = \lambda_2 = \cdots = \lambda_n = 1$.

(c) Let $\underline{w}_i$ for $i = 1, 2, ..., n$ be any $n \times 1$ vectors satisfying

$$\underline{w}_i = \begin{cases} 1, & \text{if } i = j. \\ 0, & \text{if } i \neq j. \end{cases}$$

Define $B = \sum_{i=1}^{k} \underline{w}_i \underline{w}_i'$ (note $k \leq n$), and let W be the $n \times n$ matrix whose i^{th} row is $\underline{w}_i'$. Evaluate WBW'. Hence, find the rank of B, its eigenvalues and corresponding eigenvectors.

$$WBW^T = W \left(\sum_{i=1}^{k} \underline{w}_i \underline{w}_i^T \right) W^T = \sum_{i=1}^{k} W \underline{w}_i \underline{w}_i^T W^T.$$

Now, $\underline{w}_i^T W^T = \underline{w}_i^T (\underline{w}_1, \underline{w}_2, ..., \underline{w}_n) = \overbrace{(0, 0, ..., 0, \overbrace{1,}^{i^{th}} 0, ..., 0)}^{\underline{e}_i^T}$. So,

$$WBW^T = \sum_{i=1}^{k} \underline{e}_i \underline{e}_i^T = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 1 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} = \left(\begin{array}{c|c} I_k & 0 \\ --- & --- \\ 0 & 0 \end{array} \right) \Rightarrow r(B) = r(WBW^T) = k.$$

This looks like the result mentioned in the second sentence of the problem. If so, then the $\underline{w}_i$'s are eigenvectors. Check:

$$B\underline{w}_j = \sum_{i=1}^{k} \underline{w}_i \underline{w}_i^T \underline{w}_j = \begin{cases} \underline{w}_i, & \text{if } j = i. \\ \underline{0}, & \text{otherwise.} \end{cases}$$

Hence, we can conclude that $\underline{w}_1, \underline{w}_2, ..., \underline{w}_k$ are eigenvectors with eigenvalues of 1 and that $\underline{w}_{k+1}, \underline{w}_{k+2}, ..., \underline{w}_n$ are eigenvectors with eigenvalues of 0.

(d) If in (c), you have $k = n$, what is B? Explain. If B is idempotent, it will follow from (b) that $B = I$.

$$BB = \left(\sum_{i=1}^{n} \underline{w}_i \underline{w}_i^T \right) \left(\sum_{j=1}^{n} \underline{w}_j \underline{w}_j^T \right) =$$

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \underline{w}_i \overbrace{\underline{w}_i^T \underline{w}_j}^{1 \text{ if } i=j} \underline{w}_j^T = \sum_{i=1}^{n} \underline{w}_i \underline{w}_i^T = B.$$

5. Let $\underline{x}$ be a 3×1 random vector with a $N(\underline{\mu}, I)$ distribution. Here $\underline{\mu} = (1, 1, 2)'$. Let A_1 and A_2 be the matrices

$$A_1 = \frac{1}{3} \begin{pmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix} \text{ and } A_2 = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}.$$

The theorems stated in answering the parts of this problem should be different from that given as the answer to Problem 1. First check that $A_1^2 = A_1, A_2^2 = A_2$, and $A_1 A_2 = 0$. Since $V = I$, it follows immediately that $A_1 V$ and $A_2 V$ are idempotent, and that $A_1 V A_2 = 0$.

(a) Specify completely the distribution of $y_1 = \underline{x}'A_1\underline{x}$, stating the theorem that allows you to do so. Also, specify completely the distribution of $y_2 = \underline{x}'A_2\underline{x}$. State Theorem 2.4. $y_1 \sim \chi^{2'}\left(r(A_1), \frac{1}{2}\underline{\mu}^T A_1 \underline{\mu}\right) \sim \chi^2(1)$. $y_2 \sim \chi^{2'}\left(r(A_2), \frac{1}{2}\underline{\mu}^T A_2 \underline{\mu}\right) \sim \chi^{2'}\left(1, \frac{9}{2}\right)$.

(b) Prove that y_1 and y_2 are independent, stating the theorem that allows you to do so. State Theorem 2.6. Since $A_1 V A_2 = 0$, y_1 and y_2 are independent.

(c) Let $\underline{y}_3 = B\underline{x}$ be the 2×1 random vector found by multiplying $\underline{x}$ by the matrix

$$B = \begin{pmatrix} 0 & 1 & 1 \\ 2 & 1 & -1 \end{pmatrix}.$$

Specify completely the distribution of $\underline{y}_3$. $\underline{y}_3 = B\underline{x}$ is two linearly independent combinations of a multivariate normal. So is itself multivariate normal (bivariate normal). Its distribution is then specified by its mean vector and variance matrix.

$$E(\underline{y}_3) = BE(\underline{x}) = \begin{pmatrix} 3 \\ 1 \end{pmatrix}, \quad Var(\underline{y}_3) = BVar(\underline{x})B^T = \begin{pmatrix} 2 & 0 \\ 0 & 6 \end{pmatrix}.$$

So,

$$\underline{y}_3 \sim N\left(\begin{pmatrix} 3 \\ 1 \end{pmatrix}, \begin{pmatrix} 2 & 0 \\ 0 & 6 \end{pmatrix}\right)$$

(d) Determine whether or not $\underline{y}_3$ is independent of y_1, stating the theorem that allows you to do so. State Theorem 2.5. $BVA_1 = BA_1 \neq 0 \Rightarrow$ dependence.

15.13 Full Rank Model Regression

By a *linear model* for a set of observations, we mean that the observations can be expressed as linear combinations of an unknown set of parameters plus a random error term. If we do not have full rank, then we have an ANOVA model as opposed to a regression model.

Example: Suppose the final exam scores in STAT 130 are the dependent variable y. We may think that y is related to x_1, the mid-term scores and x_2, the quiz averages. If we think the relation is approximately a linear model, then $y = a + b_1 x_1 + b_2 x_2 + \epsilon$ where ϵ is a random variable. If we have a sample of n STAT 130 students, we write the model for student i as $y_i = a + b_1 x_{i1} + b_2 x_{i2} + \epsilon_i$ or as $y_i = b_0 x_{i0} + b_1 x_{i1} + b_2 x_{i2} + \epsilon_i$, $i = 1, 2, ..., n$ where $x_{i0} = 1, \forall i$ and $b_0 = a$. The initial problem is to estimate b_0, b_1 and b_2. Generalizing, if we have k *independent variables,* $x_1, x_2, ..., x_k$ with which to model the *dependent variable* y, we can postulate the linear model $y_i = b_0 x_{i0} + b_1 x_{i1} + \cdots + b_k x_{ik} + \epsilon_i$, $i = 1, 2, ..., N$. To put this in matrix notation,

$$\underline{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}_{N\times 1} \quad X = \begin{pmatrix} x_{10} & x_{11} & x_{12} & \cdots & x_{1k} \\ x_{20} & x_{21} & x_{22} & \cdots & x_{2k} \\ x_{30} & x_{31} & x_{32} & \cdots & x_{3k} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{N0} & x_{N1} & x_{N2} & \cdots & x_{Nk} \end{pmatrix}_{N\times(k+1)} \quad \underline{b} = \begin{pmatrix} b_0 \\ b_1 \\ b_2 \\ \vdots \\ b_k \end{pmatrix}_{(k+1)\times 1} \quad \underline{e} = \begin{pmatrix} e_1 \\ e_2 \\ e_3 \\ \vdots \\ e_N \end{pmatrix}_{N\times 1}$$

So, the model is $\underline{y}_{N\times 1} = X_{N\times(k+1)}\underline{b}_{(k+1)\times 1} + \underline{e}_{N\times 1}$. We now assume the errors $\underline{e}$ satisfy

1. $E(\underline{e}) = \underline{0}$. If not, then put $\underline{e}$ into the $\underline{b}_0$ vector.
2. $Var(\underline{e}) = V$ and is positive definite.

So, $E(\underline{y}) = X\underline{b}, Var(\underline{y}) = V$. The main problem is to estimate linear functions of $\underline{b}$. We say we have a *regression model* or *full rank model* when $r(X)$ is equal to the number of columns in X or $r(X) = k+1$. Since X is $N \times (k+1)$, this implies that $N \geq k+1$. This is the topic of Chapter 3 in the text book. Later we will deal with $r(X) < k+1$. We will find the best linear unbiased estimators (B.L.U.E.S.) of $\underline{b}$. That is we want to estimate $\underline{q}^T\underline{b}$. We must find $\underline{\lambda}$ so that $E(\underline{\lambda}^T\underline{y}) = \underline{q}^T\underline{b}$ which says it is an unbiased linear estimator. By "best" we mean, $Var(\underline{\lambda}^T\underline{y})$ is minimal (smallest). Now, $E(\underline{\lambda}^T\underline{y}) = \underline{\lambda}^T E(\underline{y}) = \underline{\lambda}^T X\underline{b} = \underline{q}^T\underline{b}, \forall \underline{b}$ iff $\underline{\lambda}^T X = \underline{q}^T$. $Var(\underline{\lambda}^T\underline{y}) = \underline{\lambda}^T V\underline{\lambda}$. So, we minimize $\underline{\lambda}^T V\underline{\lambda}$ subject to $\underline{\lambda}^T X = \underline{q}^T$. Let $2\underline{\theta}$ be a vector of Lagrange multipliers. Define $F = \underline{\lambda}^T V\underline{\lambda} - 2(\underline{\lambda}^T X - \underline{q}^T)\underline{\theta}$. $\frac{1}{2}\frac{dF}{d\theta} = V\underline{\lambda} - X\underline{\theta} = \underline{0} \Rightarrow \underline{\lambda} = V^{-1}X\underline{\theta} \Rightarrow \underline{\lambda}^T = \underline{\theta}^T X^T V^{-1}$ because V is symmetric $\underline{\lambda}^T X = \underline{\theta}^T X^T V^{-1} X = \underline{q}^T \Rightarrow \underline{\theta}^T = \underline{q}^T(X^TV^{-1}X)^{-1}$. Therefore, $\underline{\lambda}^T = \underline{q}^T(X^TV^{-1}X)^{-1}X^TV^{-1}$. So, the B.L.U.E. of $\underline{q}^T\underline{b}$ is $\underline{q}^T(\underline{\lambda}^T V^{-1}X)^{-1}X^TV^{-1}$. Taking

$$\underline{q} = \underline{e}_i = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \\ 0 \end{pmatrix}$$

the B.L.U.E. of $\underline{q}^T\underline{b} = b_i$ is the i-th element of $(X^TV^{-1}X)^{-1}X^TV^{-1}\underline{y}$. We say that this is the B.L.U.E. of $\underline{b}$.

Hence, write $\widehat{\underline{b}} = (X^TV^{-1}X)^{-1}X^TV^{-1}Y$. Note that $Var(\widehat{\underline{b}}) = (X^TV^{-1}X)^{-1}\overbrace{X^TV^{-1}\overbrace{VV^{-1}}^{=I}X(X^TV^{-1}X)^{-1}}^{=I}$. Thus, $Var(\widehat{\underline{b}}) = (X^TV^{-1}X)^{-1}$.

Theorem 3.1: (Gauss) $\widehat{\underline{b}}$ minimizes $(\underline{y} - X\underline{b})^TV^{-1}(\underline{y} - X\underline{b}) = S$ with respect to $\underline{b}$ where the weights V^{-1} come from the variances and covariances and S is called a *generalized sum of squares of errors.* proof: $S = \underline{y}^TV^{-1}\underline{y} - 2\underline{b}^TX^TV^{-1}\underline{y} + \underline{b}^TX^TV^{-1}X\underline{b}$. $\frac{1}{2}\frac{dS}{d\underline{b}} = -X^TV^{-1}\underline{y} + X^TV^{-1}X\underline{b} = \underline{0} \Rightarrow X^TV^{-1}X\underline{b} = X^TV^{-1}\underline{y} \Rightarrow \widehat{\underline{b}} = (X^TV^{-1}X)^{-1}X^TV^{-1}\underline{y}$ are called the *normal equations.* $\widehat{\underline{b}}$ is the *generalized least squares estimator (GLSE).*

Theorem 3.1: (Markov) Put $\widehat{S} = \widehat{s} = (\underline{y} - X\widehat{\underline{b}})^TV^{-1}(\underline{y} - X\widehat{\underline{b}})$. Then, $E(\widehat{s}) = N - r(X)$. proof: $\underline{y} - X\widehat{\underline{b}} = \underline{y} - X(X^TV^{-1}X)^{-1}X^TV^{-1}\underline{y} = [I - X(X^TV^{-1}X)^{-1}V^TV^{-1}]\underline{y} \Rightarrow \widehat{s} = \underline{y}^T[I - V^{-1}X(X^TV^{-1}X)^{-1}X^T]V^{-1}[I - X(X^TV^{-1}X)^{-1}X^TV^{-1}]\underline{y} = \underline{y}^T[V^{-1} - V^{-1}X(X^TV^{-1}X)X^TV^{-1} - V^{-1}X(X^TV^{-1}X)^{-1}X^TV^{-1} + V^{-1}X(X^TV^{-1}X)^{-1}X^TV^{-1}X(X^TV^{-1}X)^{-1}X^TV^{-1}]\underline{y} = \underline{y}^T[V^{-1} - V^{-1}X(X^TV^{-1}X)^{-1}X^TV^{-1}]\underline{y} = \underline{y}^TA\underline{y}$ where matrix $A = V^{-1} - V^{-1}X(X^TV^{-1}X)^{-1}X^TV^{-1}$. Then, $E(\widehat{s}) = E(\underline{y}^TA\underline{y}) = tr(AV) + \underline{\mu}^TA\underline{\mu}$ where $\underline{\mu} = X\underline{b}$. Then, $AV = I - V^{-1}X(X^TV^{-1}X)^{-1}X^T$. And, $(AV)^2 = I - 2V^{-1}X(X^TV^{-1}X)^{-1}X^T + V^{-1}X(X^TV^{-1}X)^{-1}X^TV^{-1}X(X^TV^{-1}X)^{-1}X^T = I - V^{-1}X(X^TV^{-1}X)^{-1}X^T = AV$. Thus, AV is idempotent. Thus, $I - AV$ is idempotent. Thus, $tr(I) - tr(V^{-1}X(X^TV^{-1}X)^{-1}X^T) = N - tr(X^TV^{-1}X(X^TV^{-1}X)) = N = tr(I_{k+1}) = N - (k+1) = N - r(X)$. Also, $tr(AV) = tr(I_{N\times r}) - tr(V^{-1}X(X^TV^{-1}X)^{-1}X^T) = N - r(V^{-1}X(X^TV^{-1}X)^{-1}X^T) = N - r(X) = N - (k+1)$. Now, for the $\underline{\mu}^TA\underline{\mu}$. $\underline{\mu}^TA\underline{\mu} = \underline{b}^TX^T[V^{-1} - V^{-1}X(X^TV^{-1}X)^{-1}X^TV^{-1}]X\underline{b} = \underline{b}^TX^TV^{-1}X\underline{b} - \underline{b}^TX^TV^{-1}X(X^TV^{-1}X)^{-1}X^TV^{-1}X\underline{b} = \underline{b}^TX^TV^{-1}X\underline{b} - \underline{b}^TX^TV^{-1}X\underline{b} = 0$. Hence, we have the B.L.U.E. of $\underline{b}$ and we know that it minimizes the generalized sum of square of errors. Theorem 3.2 gives the expected value of the error sum of squares. In particular, if $V = \sigma^2R$ where R is known, then

$$E\left[\frac{(\underline{y} - X\underline{b})^TR^{-1}(\underline{y} - X\underline{b})}{N - r(X)}\right] = \sigma^2.$$

An important special case arises when $V = \sigma^2 I$. We have $V^{-1} = \sigma^{-2} I \Rightarrow \widehat{\underline{b}} = (X^T V^{-1} X)^{-1} X^T V^{-1} \underline{y} = (X^T X)^{-1} X^T \underline{y}$. Then, $Var(\widehat{\underline{b}}) = (X^T V^{-1} X)^{-1} = (X^T \sigma^2 I X)^{-1} = \sigma^2 (X^T X)^{-1}$. Write $\widehat{\underline{y}} = X\widehat{\underline{b}}$ as the estimate of $E(\underline{y}) = X\underline{b}$. Then, $\widehat{\underline{y}} = X(X^T X)^{-1} X^T \underline{y} = P_X \underline{y}$ where $P_{\underline{x}}$ projects onto $\varrho(X)$. Define $SS(E) = \sigma^2 \widehat{S} = (\underline{y} - \widehat{\underline{y}})^T (\underline{y} - \widehat{\underline{y}}) = (\underline{y} - P_x \underline{y})^T (\underline{y} - P_X \underline{y}) = \underline{y}^T (I - P_x)^T (I - P_x) \underline{y} = \underline{y}^T (I - P_x)(I - P_x) \underline{y} = \underline{y}^T (I - P_x) \underline{y}$. Therefore, $\frac{SS(E)}{N - r(X)}$ is an unbiased estimator of σ^2.
The model statement is $\underline{y}_{N\times 1} = X_{N\times(k+1)} \underline{b}_{(k+1)\times 1} + \underline{e}_{N\times 1}$ where $E(\underline{e}) = \underline{0}$ and $Var(\underline{e}) = V$ and is a positive definite matrix. $\widehat{\underline{b}} = (X^T V^{-1} X)^{-1} X^T V^{-1} \underline{y}$. A special case of the variance is $V = \sigma^2 I$. Then, the parameter estimates become $\widehat{\underline{b}} = (X^T V^{-1} X)^{-1} X^T V^{-1} \underline{y} = (X^T \frac{1}{\sigma^2} X)^{-1} X^T \frac{1}{\sigma^2} I \underline{y} = (X^T X)^{-1} X^T \underline{y}$. The variances of the parameter estimates are $Var(\widehat{\underline{b}}) = (X^T V^{-1} X)^{-1} = (X^T \frac{1}{\sigma^2} I X)^{-1} = \sigma^2 (X^T X)^{-1}$. $\widehat{\underline{y}} = X\widehat{\underline{b}} = X(X^T X)^{-1} X^T \underline{y} = P_X \underline{y}$ where P_X projects onto the column space $\varrho(X)$. $\widehat{s} = (\underline{y} - X\widehat{\underline{b}})^T V^{-1} (\underline{y} - X\widehat{\underline{b}}) = \frac{1}{\sigma^2} (\underline{y} - P_X \underline{y})^T (\underline{y} - P_X \underline{y}) = \frac{1}{\sigma^2} \underline{y}^T (I - P_X)^T (I - P_X) \underline{y} = \frac{1}{\sigma^2} \underline{y}^T (I - P_X) \underline{y}$ because of idempotency. Define $SS(E) = \sigma^2 \widehat{s} = \underline{y}^T (I - P_X) \underline{y}$. Then by Theorem 3.2, $E(SS(E)) = \sigma^2 (N - r(X))$. So, $SS(E)/(N - r(X))$ is an unbiased estimate for σ^2.

15.13.1 Distributional Properties

Let now assume that $\underline{e} \sim N(\underline{0}, V)$ i.e. $\underline{y} \sim N(X\underline{b}, V)$. So,

$$f_{\underline{y}}(\underline{y}) = \frac{1}{(2\pi)^{N/2} |V|^{\frac{1}{2}}} \exp\left\{ -\frac{1}{2} (\underline{y} - X\underline{b})^T V^{-1} (\underline{y} - X\underline{b}) \right\}$$

Consider this as a likelihood function $L(\underline{b}, \underline{y})$ for $\underline{b}$. The mle for $\underline{b}$ is the $\widehat{\underline{b}}$ which maximizes the likelihood i.e. the one that minimizes the quadratic form $(\underline{y} - X\underline{b})^T V^{-1} (\underline{y} - X\underline{y}) = s$. Theorem 3.1 says that this $\widehat{\underline{b}}$ is the one we already have. The mle, B.L.U.E., and G.L.S.E. is $\widehat{\underline{b}} = (X^T V^{-1} X)^{-1} X^T V^{-1} \underline{y}$. Also, $\widehat{\underline{b}} \sim N(\underline{b}, (X^T V^{-1} X)^{-1})$. $\widehat{s} = \underline{y}^T A \underline{y}$. For matrix A, see proof of Theorem 3.2. In that proof, we showed that AV was idempotent and $(X\underline{b})^T A (X\underline{b}) = \underline{0}$. $\widehat{s} \sim \chi^2[N - r(X), 0]$. For $V = \sigma^2 I$, this reduces to $\widehat{\underline{b}} \sim N(\underline{b}, \sigma^2 (X^T X)^{-1})$ and $SS(E)/\sigma^2 \sim \chi^2[N - r(X)]$.

15.13.2 Tests of Hypotheses

In general, linear hypotheses of order s specifies the value of s linearly independent linear combinations of the elements of $\underline{b}$. Hence, it may be written as $K^T_{s\times(k+1)} \underline{b}_{(k+1)\times 1} = \underline{m}_{s\times 1}$ where $r(X) = s$. This is no restriction on generality. We assume that $\underline{y} \sim N(X\underline{b}, \sigma^2 I)$, $\underline{e} \sim N(\underline{0}, \sigma^2 I)$ in the model $\underline{y} = X\underline{b} + \underline{e}$. We wish to find the likelihood ratio statistic for testing $H_0 : K^T \underline{b} = \underline{m}$ versus $H_1 : K^T \underline{b} \neq \underline{m}$. The general form of a likelihood ratio test statistic is

$$L(\underline{y}) = \frac{\max_{H_0} f_{\underline{y}}(\underline{y})}{\max f_{\underline{y}}(\underline{y})}.$$

H_0 is reject if L is too small.

$$f_{\underline{y}}(\underline{y}) = \frac{1}{(2\pi)^{N/2} \sigma^N} \exp\left\{ -\frac{1}{2\sigma^2} (\underline{y} - X\underline{b})^T (\underline{y} - X\underline{b}) \right\}$$

Equivalently we maximize

$$\log f_{\underline{y}}(\underline{y}) = -\frac{N}{2} \log(2\pi) - N \log\sigma - \frac{1}{2\sigma^2} (\underline{y} - X\underline{b})^T (\underline{y} - X\underline{b}).$$

$$\frac{\partial \log f}{\partial \sigma} = -\frac{N}{\sigma} + \frac{1}{\sigma^3}(\underline{y} - X\underline{b})^T(\underline{y} - X\underline{b}) = 0 \Rightarrow \frac{(\underline{y} - X\underline{b})^T(\underline{y} - X\underline{b})}{N} = \widehat{\sigma} \Rightarrow \widehat{\sigma} = \frac{SS(E)}{N} \Rightarrow$$

$$\max f_{\underline{y}}(\underline{y}) = \frac{1}{(2\pi)^{N/2}\left(\frac{SS(E)}{N}\right)^{N/2}} \exp\left\{-\frac{1}{2\frac{SS(E)}{N}}SS(E)\right\} = \left(\frac{2\pi e}{N}\right)^{-N/2}(SS(E))^{-N/2}.$$

Similarly we see that

$$\max_{H_0} f_{\underline{y}}(\underline{y}) = \left(\frac{2\pi e}{N}\right)^{-N/2}(SS_0)^{-N/2}$$

where $SS_0 = \min_{H_0}(\underline{y} - X\underline{b})^T(\underline{y} - X\underline{b})$. So, the likelihood function is

$$L(\underline{y}) = \frac{SS_0^{-N/2}}{SS(E)^{-N/2}} = \left(\frac{SS_0}{SS(E)}\right)^{-N/2}.$$

We reject H_0 if

1. $L \leq c$.
2. $L^{-1} \geq c_0$.
3. $\left(\frac{SS_0}{SS(E)}\right)^{N/2} \geq c_0$.
4. $\left(\frac{SS_0}{SS(E)}\right) \geq c_1 = c_0^{2/N}$.
5. $\left(\frac{SS_0}{SS(E)}\right) - 1 \geq c_2 = c_1 - 1$.
6. $\left(\frac{SS_0 - SS(E)}{SS(E)}\right) \geq c_2$.
7. $\frac{Q}{SS(E)}\frac{(N-r(X))}{s} \geq c_3 = \left(\frac{N-r(X)}{s}\right)c_2$ where $Q = SS_0 - SS(E)$.

Let $2\underline{\theta}$ be a vector of Lagrange multipliers and write $F = \underline{y}^T\underline{y} - 2\underline{b}^T X^T\underline{y} + \underline{b}^T X^T X\underline{b} + 2(\underline{b}^T K - \underline{m}^T)\underline{\theta}$. $\frac{1}{2}\frac{\partial F}{\partial \underline{b}} = -X^T\underline{y} + X^T X\underline{b} + K\underline{\theta} = \underline{0} \Rightarrow X^T X\underline{\tilde{b}} = X^T\underline{y} - K\underline{\theta} \Rightarrow \tilde{b} = (X^T X)^{-1}X^T\underline{y} - (X^T X)^{-1}K\underline{\theta} = \underline{\widehat{b}} - (X^T X)^{-1}K\underline{\theta} \Rightarrow (X^T X)^{-1}K\underline{\theta} = \underline{\widehat{b}} - \underline{\tilde{b}} \Rightarrow K^T(X^T X)^{-1}K\underline{\theta} = K^T(\underline{\widehat{b}} - \underline{\tilde{b}}) \Rightarrow \underline{\theta} = (K^T(X^T X)^{-1}K)^{-1}K^T(\underline{\widehat{b}} - \underline{\tilde{b}}) = (K^T(X^T X)^{-1}K)^{-1}(K^T\underline{\widehat{b}} - \underline{m}) \Rightarrow \underline{\tilde{b}} = \underline{\widehat{b}} - (X^T X)^{-1}K(K^T(X^T X)^{-1}K)^{-1}(K^T\underline{\widehat{b}} - \underline{m})$. Hence, $SS_0 = (\underline{y} - X\underline{\tilde{b}})^T(\underline{y} - X\underline{\tilde{b}}) = [(\underline{y} - X\underline{\widehat{b}} + X(\underline{\widehat{b}} - \underline{\tilde{b}})]^T[(\underline{y} - X\underline{\widehat{b}} + X(\underline{\widehat{b}} - \underline{\tilde{b}})] = (\underline{y} - X\underline{\widehat{b}})^T(\underline{y} - X\underline{\widehat{b}}) + 2(\underline{\widehat{b}} - \underline{\tilde{b}})^T \overbrace{X^T(\underline{y} - X\underline{\widehat{b}})}^{=0} + (\underline{\widehat{b}} - \underline{\tilde{b}})^T X^T X(\underline{\widehat{b}} - \underline{\tilde{b}}) = SS(E) + (\underline{\widehat{b}} - \underline{\tilde{b}})^T(X^T X)(\underline{\widehat{b}} - \underline{\tilde{b}}) \Rightarrow Q = SS_0 - SS(E) = (\underline{\widehat{b}} - \underline{\tilde{b}})^T(X^T X)(\underline{\widehat{b}} - \underline{\tilde{b}}) \Rightarrow Q = (K^T\underline{\widehat{b}} - \underline{m})^T(K^T(X^T X)^{-1}K)^{-1}\ K^T(X^T X)^{-1}(X^T X)K(K^T(X^T X)^{-1}K)^{-1}(K^T\underline{\widehat{b}} - \underline{m}) = (K^T\underline{\widehat{b}} - \underline{m})^T(K^T(X^T X)^{-1}K)^{-1}(K^T\underline{\widehat{b}} - \underline{m})$. We call this expression the *sums of squares for testing* H_0.

15.13.3 Likelihood Ratio Test

See the previous subsection for an introduction to this section. The likelihood ratio test of $H : K^T\underline{b} = \underline{m}$ has the test statistic of the form $\frac{Q}{SS(E)}\frac{N-r(X)}{S}$ where $Q = SS_0 - SS(E)$ where the sums of squares are restricted by the hypothesis above and $SS_0 = \min_{K^T\underline{b}=\underline{m}}\left\{(\underline{y} - X\underline{b})^T(\underline{y} - X\underline{b})\right\}$. $Q = (K^T\underline{\widehat{b}} - \underline{m})^T(K^T(X^T X)^{-1}K)^{-1}(K^T\underline{\widehat{b}} - \underline{m})$. Let's find the distribution of Q. We know that $K^T\underline{\widehat{b}} - \underline{m} = K^T(X^T X)^{-1}X^T\underline{y}X^T\underline{y} - \underline{m}$ are linear combinations of the multinomial $E(K^T\widehat{\underline{b}} - \underline{m}) = K^T\underline{b} - \underline{m}$ due to un-biasness. Then, $Var(K^T\underline{b} - \underline{m}) = Var(K^T\widehat{\underline{b}}) = \sigma^2 K^T(X^TX)^{-1}K$. Therefore, $K^T\widehat{\underline{b}} - \underline{m} \sim N(K^T\underline{b} - \underline{m}, \sigma^2 K^T(X^TX)^{-1}K)$. We want the matrix of the quadratic and the variance to be idempotent. Therefore, choose $\frac{Q}{\sigma^2} \sim \chi^{2'}[S, \frac{1}{2}\frac{1}{\sigma^2}(K^T\underline{b} - \underline{m})(K^T(X^TX)^{-1}K)^{-1}(K^T\underline{b} - \underline{m})]$. Finally, show that Q and $SS(E)$ are independent. $\frac{SS(E)}{\sigma^2} = \underline{y}^T\frac{(I-P_x)}{\sigma^2}\underline{y}$. $P_x = X(X^TX)^{-1}X^T$ projects onto $\varrho(X)$. Let $A_1 = \frac{(I-P_x)}{\sigma^2}$. We need to also express Q as a quadratic for in $\underline{y}$. $K^T\widehat{\underline{b}} - \underline{m} = K^T(X^TX)^{-1}X^T\underline{y} - \underline{m}$. $\frac{Q}{\sigma^2} = \left[K^T(X^TX)^{-1}X^T\underline{y} - \underline{m}]^T(K^T(X^TX)^{-1}K)^{-1}[K^T(X^TX)^{-1}X^T\underline{y} - \underline{m}]\right]\Big/\sigma^2$. The matrix A_2 of the quadratic form Q, when expressed as a quadratic function in $\underline{y}$ is $A_2 = \frac{1}{\sigma^2}\ X(X^TX)^{-1}K\ (K^T(X^TX)^{-1}\ K)^{-1}\ K^T\ (X^TX)^{-1}X^T$. Then, $\frac{SS(E)}{\sigma^2}$ and $\frac{Q}{\sigma^2}$ are independent iff $A_1 \cup A_2 = 0$ by Theorem 2.6. Here, where $V = \sigma^2 I$ and it also implies that $A_1A_2 = 0$. $A_1A_2 = \frac{1}{\sigma^2}(I - P_x)(X(X^TX)^{-1}K(K^T(X^TX)^{-1}K)^{-1}K^T \cdots . \Rightarrow 0 \times [\cdots] = 0$.

Theorem 3.3: Let $\underline{y} = X\underline{b} + \underline{e}$ where $\underline{e} \sim N(\underline{0}, \sigma^2 I)$ and X has full column rank. The likelihood ratio test statistic for the general linear hypothesis $H: K^T\underline{b} = \underline{m}$ (K has full column rank) is

$$L = \frac{(K^T\widehat{\underline{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1}(K^T\widehat{\underline{b}} - \underline{m})/r(K)}{(\underline{y} - X\widehat{\underline{b}})^T(\underline{y} - X\widehat{\underline{b}})/(N - r(X))}.$$

The distribution of L is $L \sim F'\left[r(K), N - r(X), \frac{1}{2\sigma^2}(K^T\underline{b} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1}(K\underline{b} - \underline{m})\right]$. Hence, we reject iff $L > F[r(K), N - r(X), 1 - \alpha]$. There are two useful facts about this derivation.

1. We calculated the quantity $SS_0 = \min(\underline{y} - X\underline{b})^T(\underline{y} - X\underline{b}) = (\underline{y} - X\tilde{\underline{b}})^T(\underline{y} - X\tilde{\underline{b}})$. This is actually the squared errors for the *reduced model* obtained by imposing the restriction $K^T\underline{b} = \underline{m}$ on $\underline{b}$. Hence, we call it $SS(E)$ reduced. We have $SS(E)_{\text{reduced}} = (\underline{y} - X\tilde{\underline{b}})^T(\underline{y} - X\tilde{\underline{b}}) = Q + SS(E)_{\text{full}}$. So, Q is the difference between the $SS(E)_{\text{reduced}}$ and the $SS(E)_{\text{full}}$. More will be said about this later.

2. The estimate of $\underline{b}$ in the reduced model is $\tilde{\underline{b}} = \widehat{\underline{b}} - (X^TX)^{-1}K(K^T(X^TX)^{-1}K)^{-1}(K^T\widehat{\underline{b}} - \underline{m})$ from a previous lecture.

Here are some important special cases of Theorem 3.3.

1. $H: \underline{b} = \underline{0}, (\underline{y} = \underline{e})$. Then, $K^T = I$ and $\underline{m} = \underline{0}$. So, $Q = (K^T\widehat{\underline{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1}(K^T\widehat{\underline{b}} - \underline{m}) = \widehat{\underline{b}}^T(X^TX)\widehat{\underline{b}}$, where $\widehat{\underline{b}} = (X^TX)^{-1}X^T\underline{y}$. Then, $Q = \underline{y}^TX(X^TX)^{-1}(X^TX)(X^TX)^{-1}X^T\underline{y} = \underline{y}^TP_x\underline{y}$ or it can be written as $(P_x\underline{y})^T(P_x\underline{y})$ or as $\underline{y}^T\underline{y} = SS(R)$ which is the sums of squares for regression. Note: $SS(E) + SS(R) = \underline{y}^T(I - P_x)\underline{y} + \underline{y}^TP_x\underline{y} = \underline{y}^T\underline{y} = SS(TOT)$ which is the total sums of squares.

2. $H: \underline{b} = \underline{b}_0$ where $\underline{b}_0$ is a vector of specified constants. Now, $K^T = I, \underline{m} = \underline{b}_0$ and we get $Q = (\widehat{\underline{b}} - \underline{b}_0)^T(X^TX)(\widehat{\underline{b}} - \underline{b}_0)$. Case (1): Special case of this with $\underline{b}_0 = \underline{0}$. Note that the estimate of $\underline{b}$ under the reduced model is $\tilde{\underline{b}} = \widehat{\underline{b}} - (X^TX)^{-1}K(K^T(X^TX)^{-1}K)^{-1}(K^T\widehat{\underline{b}} - \underline{m})$. The following model completely specifies the $\underline{b}$ estimate: $\tilde{\underline{b}} = \widehat{\underline{b}} - (\widehat{\underline{b}} - \underline{b}_0) = \underline{b}_0$.

3. $H: \underline{\lambda}^T\underline{b} = m$ for some vector $\underline{\lambda}^T = (\lambda_0, \lambda_1, ..., \lambda_k)$, and $K^T = \underline{\lambda}^T$, $\underline{m} = m$, $s = 1$, and $Q = (\underline{\lambda}^T\widehat{\underline{b}} - m)^T(\underline{\lambda}^T(X^TX)^{-1}\underline{\lambda})^{-1}(\underline{\lambda}^T\widehat{\underline{b}} - m) = \frac{(\underline{\lambda}^T\widehat{\underline{b}} - m)^2}{\underline{\lambda}^T(X^TX)^{-1}\underline{\lambda}}$ which is going to be a t statistic. The estimator of $\underline{b}$ under the reduced model is $\tilde{\underline{b}} = \widehat{\underline{b}} - (X^TX)^{-1}\underline{\lambda}(\underline{\lambda}^T(X^TX)^{-1}\underline{\lambda})^{-1}(\underline{\lambda}^T\widehat{\underline{b}} - m) = \widehat{\underline{b}} - \frac{(\underline{\lambda}^T\widehat{\underline{b}} - m)^2}{\underline{\lambda}^T(X^TX)^{-1}\underline{\lambda}}(X^TX)^{-1}\underline{\lambda}$.

4. Partition $\underline{b}$ as

$$\underline{b} = \begin{pmatrix} \underline{b}_q \\ \cdots \\ \underline{b}_p \end{pmatrix}$$

where $\underline{b}_q^T = (b_0, b_1, ..., b_{q-1})$ is the first q elements of $\underline{b}$. The hypothesis is $H : \underline{b}_q = \underline{0}$. It states that the first q random variables are irrelevant. So, $s = q, \underline{m} = \underline{0}_{q\times 1}$, and $K^T_{q\times(k+1)} = [I_q \ : \ 0]$. Make the corresponding partition of $\widehat{\underline{b}}$ and of $(X^TX)^{-1}$

$$\widehat{\underline{b}} = \begin{pmatrix} \widehat{\underline{b}}_q \\ \cdots \\ \widehat{\underline{b}}_p \end{pmatrix} \text{ and } (X^TX)^{-1} = \begin{pmatrix} T_{qq} & \vdots & T_{qp} \\ \cdots & \cdots & \cdots \\ T_{pq} & \vdots & T_{pp} \end{pmatrix}.$$

Then, $K^T\widehat{\underline{b}} = \widehat{\underline{b}}_q$ and $Q = (K^T\widehat{\underline{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1}(K^T\widehat{\underline{b}} - \underline{m}) = (\widehat{\underline{b}}_q)^T T_{qq}^{-1}\widehat{\underline{b}}_q$ where T_{qq}^{-1} is the inverse of the part of $(X^TX)^{-1}$ corresponding to the variables being tested and $\widehat{\underline{b}}_q$ is an estimate of the b's corresponding to the variables being tested. This works, in general, for testing any subset of the b_i's equal to 0. We choose the first q's for convenience only. The estimate of $\underline{b}$ in the reduced model is

$$\tilde{\underline{b}} = \widehat{\underline{b}} - (X^TX)^{-1}K(K^T(X^TX)^{-1}K)^{-1}(K^T\widehat{\underline{b}} - \underline{m}) =$$

$$\begin{pmatrix} \widehat{\underline{b}}_q \\ \cdots \\ \widehat{\underline{b}}_p \end{pmatrix} - \begin{pmatrix} T_{qq} & \vdots & T_{qp} \\ \cdots & \cdots & \cdots \\ T_{pq} & \vdots & T_{pp} \end{pmatrix} \begin{pmatrix} I_q \\ \cdots \\ 0 \end{pmatrix} T_{qq}^{-1}\widehat{\underline{b}}_q = \begin{pmatrix} \widehat{\underline{b}}_q \\ \cdots \\ \widehat{\underline{b}}_p \end{pmatrix} - \begin{pmatrix} T_{qq} \\ \cdots \\ T_{pq} \end{pmatrix} T_{qq}^{-1}\widehat{\underline{b}}_q =$$

$$\begin{pmatrix} \widehat{\underline{b}}_q \\ \cdots \\ \widehat{\underline{b}}_p \end{pmatrix} - \begin{pmatrix} \widehat{\underline{b}}_q \\ \cdots \\ T_{pq}T_{qq}^{-1}\widehat{\underline{b}}_q \end{pmatrix} = \begin{pmatrix} \underline{0}_q \\ \cdots \\ \widehat{\underline{b}}_p - T_{pq}T_{qq}^{-1}\widehat{\underline{b}}_q \end{pmatrix}.$$

Items (1) - (4) can be found in the text book on pages 113-116.

5. As a special case of (4), suppose our model is $y = b_0 + b_1x_1 + \cdots + b_kx_k + e_k$. The first element of b is an intercept term. We write $\underline{b} = \begin{pmatrix} b_0 \\ \cdots \\ \underline{\beta} \end{pmatrix}$ where $\underline{\beta}^T = (b_1 \quad b_2 \quad \cdots \quad b_k)$ is the vector of slopes. The sum of squares for testing $H : \underline{\beta} = 0$ is $Q = \widehat{\underline{\beta}}^T S\widehat{\underline{\beta}}$ where $\widehat{\underline{\beta}} = (\widehat{\underline{b}}_1 \quad \widehat{\underline{b}}_2 \quad \cdots \quad \widehat{\underline{b}}_k)$. $Q = SS(R)_m$ is the sum of squares for regression given the mean (or intercept) and S is the inverse (known from item [4]) of the lower $k \times k$ diagonal sub-matrix of $(X^TX)^{-1}$. In the text book (equations 33-35, page 84), it is shown that $S = X_1^TX_1 - \frac{1}{n}X^Tjj^TX_1$ where $X = (j|X_1)$ where j is an $N \times 1$ vector and X_1 is an $N \times k$ matrix.

15.13.4 The Reduced Model $K^Tb = 0$.

We impose the constraint $K^T\underline{b} = 0$. on our model. Here K^T is $s \times (k+1)$ of rank s and $s \leq k$ (i.e. K^T is not square). We have $Q = \widehat{\underline{b}}^TK(K^T(X^TX)^{-1}K)^{-1}K^T\widehat{\underline{b}} = \underline{y}^T \overbrace{X(X^TX)^{-1}K(K^T(X^TX)^{-1}K)^{-1}K^T(X^TX)^{-1}X^T}^{\text{call it } A_H}\underline{y}$. A_H is called a matrix of *quadratic form*. Now, $P_xA_H = A_H$. So, $(P_x - A_H)(P_x - A_H) = P_x^2 - A_HP_x - P_xA_H + A_H^2 = P_X - A_H - A_H + A_H = P_x - A_H \Rightarrow P_x - A_H$ is idempotent and so was A_H. Also, $A_H(P_x - A_H) = A_HP_x - A_H^2 = A_H - A_H = 0$. So, the quadratic forms $\underline{y}^TA_H\underline{y}$ and $\underline{y}^T(P_x - A_H)\underline{y}$ are independent $\sigma^2\chi^2$'s which sum to $\underline{y}^TA_H\underline{y} + \underline{y}^T(P_x - A_H)\underline{y} = \underline{y}^TP_x\underline{y} = SS(R)$. We know $\underline{y}^TA_H\underline{y}$ is used to test $K^T\underline{b} = 0$ in the full model. We will show that $\underline{y}^T(P_x - A_H)\underline{y}$ tests the regression in the reduced model. We have $Q = SSE(reduced) - SSE(full)$. $\underline{y}^TA_H\underline{y} = SSE(reduced) - SSE(full) = SSE(reduced) - \underline{y}^T(I - P_x)\underline{y}$. Rearranging terms gives $\underline{y}^T(P_x - A_H)\underline{y} = \underline{y}^T\underline{y} - SSE(reduced) = SS(total) - SSE(reduced) = SS(R)_{reduced}$. Hence, $\underline{y}^T(P_x - A_H)\underline{y}$ is the regression sum of squares in the reduced model and hence tests the regression in that model. This can also be stated as follow. Let L be any matrix such that $\begin{pmatrix} K^T \\ \cdots \\ L^T \end{pmatrix}$ is

$(k+1)\times(k+1)$ or rank $k+1$. Then, $\underline{y}^T(P_x - A_H)\underline{y}$ tests $H: L^T\underline{b} = 0$ *given that* $K^T\underline{b} = 0$ (this can be derived by re-parameterization). A consequence of this is $Q = \underline{y}^T A_H \underline{y} = \underline{y}^T P_x \underline{y} - \underline{y}^T(P_x - A_H)\underline{y} = SS(R)_{full} - SS(R)_{reduced}$. So, Q is both the *decrease in* $SS(E)$ from the reduced to the full model and the *increase in* $SS(R)$ from the reduced to the full model. $SS(R)_{full} = \underline{y}^T P_x \underline{y} = \underline{y}^T A_H \underline{y} + \underline{y}^T(P_x - A_H)\underline{y}$.

$\underline{y}^T A_H \underline{y}:$

1. Gain in $SS(R)$ from the reduced to the full model.
2. Loss in $SS(E)$ from the reduced to the full model.
3. Tests $K^T\underline{b} = 0$ in the full model.

$\underline{y}^T(P_x - A_H)\underline{y}:$

1. $SSR(reduced)$ tests the regression in the reduced model.

When the reduced model is $K^T\underline{b} = \underline{m}$ for some $\underline{m} \neq 0$, $SS(R)_{reduced} \neq \underline{y}^T(P_x - A_H)\underline{y}$. So, the breakdown of $\underline{y}^T P_x \underline{y} = \underline{y}^T A_H \underline{y} + \underline{y}^T(P_x - A_H)\underline{y}$ does not have a nice interpretation in terms of full models and reduced models. What happens in the reduced model $K^T\underline{b} = \underline{m}$ when $\underline{m} \neq \underline{0}$? We have $Q = (K^T\widehat{\underline{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1}(K^T\widehat{\underline{b}} - \underline{m}) = [K^T(X^TX)^{-1}X^T\underline{y} - \underline{m}]^T(K^T(X^TX)^{-1}K)^{-1}[K^T(X^TX)^{-1}X^T\underline{y} - \underline{m}] = (\underline{y} - \underline{m}_1)^T X(X^TX)^{-1}K(K^T(X^TX)^{-1}K)^{-1}K^T(X^TX)^{-1}X^T(\underline{y} - \underline{m}_1) = (\underline{y} - \underline{m}_1)^T A_H(\underline{y} - \underline{m}_1)$ where $\underline{m}_1 = XK(K^TK)^{-1}\underline{m}$ and $A_H = X(X^TX)^{-1}K(K^T(X^TX)^{-1}K)^{-1}K^T(X^TX)^{-1}X^T$. To study the reduced model, note that $K^T\underline{b} = \underline{m} \Rightarrow XK(K^TK)^{-1}K^T\underline{b} = XK(K^TK)^{-1}\underline{m} \Rightarrow XP_K\underline{b} = \underline{m}_1$ because $K(K^TK)^{-1}K^T\underline{b} = P_k$ by Theorem 1.6. Also, by multiplying by $(X^TX)^{-1}$, this implies that $X^TXP_k\underline{b} = X^TXK(K^TK)^{-1}\underline{m} \Rightarrow P_k\underline{b} = K(K^TK)^{-1}\underline{m} \Rightarrow K^T\underline{b} = \underline{m}$ by multiplying by K^T in the last equality. So, $K^T\underline{b} = \underline{m}$ iff $XP_x\underline{b} = \underline{m}_1$. The reduced model is $\underline{y} = X\underline{b} + \underline{e}$ subject to $K^T\underline{b} = \underline{m}$ or $\underline{y} = X[P_x + (I - P_x)]\underline{b} + \underline{e}$ subject to $XP_x\underline{b} = \underline{m}_1$ or $\underline{y} = \underline{m}_1 + X(I - P_K)\underline{b} + \underline{e}$, where the restriction is now in the model. Another alternative is $\underline{y} - \underline{m}_1 = X\underline{b} + \underline{e}$ where $\underline{b} \in \varrho^{\perp}(K)$ (i.e. $K^T\underline{b} = \underline{0}$ because the left-hand-side changed) and that explains why the $SS(total)$ changes). The $SS(total)$ for this model is $(\underline{y} - \underline{m}_1)^T(\underline{y} - \underline{m}_1)$. So, $SS(R)_{reduced} = SS(total)_{reduced} - SS(E)_{reduced} = SS(total)_{reduced} - [Q + SS(E)_{full}] = (\underline{y} - \underline{m}_1)^T(\underline{y} - \underline{m}_1) - (\underline{y} - \underline{m}_1)A_H(\underline{y} - \underline{m}_1) - \underline{y}^T(I - P_x)\underline{y}$. Note that $\underline{m}_1 = XK(K^T(K^TK)^{-1}\underline{m}$ so that $(I - P_x)\underline{m}_1 = 0$. Thus, we can rewrite the statement as $(\underline{y} - \underline{m}_1)^T(\underline{y} - \underline{m}_1) - (\underline{y} - \underline{m}_1)^T A_H(\underline{y} - \underline{m}_1) - (\underline{y} - \underline{m}_1)^T(I - P_x)(\underline{y} - \underline{m}_1) \Rightarrow SS(R)_{reduced} = (\underline{y} - \underline{m}_1)^T(P_x - A_H)(\underline{y} - \underline{m}_1)$.

15.13.5 Summary

For the full model, we have the following notes.

1. $\underline{y} = X\underline{b} + \underline{e}$, $\underline{b}$ is arbitrary.
2. $SS(R)_{full} = \underline{y}^T P_x \underline{y}$.
3. $SS(E)_{full} = \underline{y}^T(I - P_x)\underline{y}$.
4. $SS(T)_{full} = \underline{y}^T\underline{y}$.

For the reduced model $K^T\underline{b} = 0$, we have the following notes.

1. $\underline{y} = X\underline{b} + \underline{e}$ where $\underline{b} \in \varrho^{\perp}(K)$.
2. $SS(R)_{reduced} = \underline{y}^T(P_x - A_H)\underline{y}$.
3. $SS(E)_{reduced} = \underline{y}^T(I - P_x + A_H)\underline{y}$.
4. $SS(T)_{reduced} = \underline{y}^T\underline{y}$.

For the reduced model $K^T\underline{b} = \underline{m}$, $\underline{m} \neq \underline{0}$, we have the following notes.

1. $\underline{y} - \underline{m}_1 = X\underline{b} + \underline{e}$ where $\underline{b} \in \varrho^{\perp}(K)$.
2. $SS(R)_{reduced} = (\underline{y} - \underline{m}_1)^T(P_x - A_H)(\underline{y} - \underline{m}_1)$.
3. $SS(E)_{reduced} = (\underline{y} - \underline{m}_1)^T(I - P_x + A_H)(\underline{y} - \underline{m}_1)$.
4. $SS(T)_{reduced} = (\underline{y} - \underline{m}_1)^T(\underline{y} - \underline{m}_1)$.

We can always write $SS(R)_{full} = \underline{y}^T A_H \underline{y} + \underline{y}^T(P_x - A_H)\underline{y} = Q + \underline{y}^T(P_x - A_H)\underline{y}$. But the second quantity has a nice interpretation in the reduced model only when the restriction has $\underline{m} = \underline{0}$. The analysis of variance for $K^T\underline{b} = \underline{0}$ is

Source	d.f.	SS	F
Regression (full)	$r = r(X)$	$\underline{y}^T P_x \underline{y}$	$\underline{y}^T P_x \underline{y}/r$
Hypothesis	s = no. rows in K^T	$\underline{y}^T A_H \underline{y} = Q$	$\frac{Q/s}{MS(E)}$
Reduced Model	$r - s$	$\underline{y}^T(P_x - A_H)\underline{y} = SS(R)_{reduced}$	$\frac{MS(R)_{reduced}}{MSE}$
Residual Error	$N - r$	$\underline{y}^T(I - P_x)\underline{y} = SS(E)$	$\frac{SS(E)}{N-r}$
Total	N (no adj for mean b_0)	$\underline{y}^T\underline{y}$	

For the reduced model $K^T\underline{b} = \underline{m}$ with $\underline{m} \neq \underline{0}$, it does not give a breakdown like in the above ANOVA table. A very common special case is our case (5) on page 1040 for hypothesis cases. Our hypothesis is $K^T\underline{b} = \underline{0}$ where $K^T = (\underline{0}_k,\ I_k)$. The hypothesis is $H_0 : b_1 = b_2 = \cdots = b_k = 0$. It says $x_1, x_2, ..., x_k$ are irrelevant. The reduced model is $\underline{y} = b_0 + e$. So, $SS(R)_{reduced}$ is called $SS(mean)$. The ANOVA table for case (5) on page 1040 is

Source	d.f.	SS
Regression (full)	$k + 1$	$SS(R) = \underline{y}^T P_x \underline{y}$
Hypothesis	k	$SS(R)_m$
Reduced	1	$SS(M)$
Residual Error	$N - (k + 1)$	$SS(E)$
Total	N	SS(T) $= \underline{y}^T\underline{y}$

Common variations on this ANOVA table include the following ANOVA table. This is the one that SAS prints.

Source	d.f.	SS
Regression (adjusted)	k	$SS(R)_m$
Residual	$N - k - 1$	$SS(E)$
Total (adj)	$N - 1$	$SS(T)_m = SS(T) - SS(M)$
Mean	1	$SS(M)$
Total	N	$SS(T) = \underline{y}^T\underline{y}$

15.14 Departure from Multi-linearity (Lack-of-Fit)

If we can obtain several measurements for the same fixed values of $(x_1, x_2, ..., x_k)$, we can test the adequacy of our regression model. The full model is $y_{ij} = b_0 + b_1x_{1i} + b_2x_{i2} + \cdots + b_kx_{ik} + \cdots + \delta_i + \cdots + e_{ij}$. The reduced model is $y_{ij} = b_0 + b_1x_{1i} + b_2x_{i2} + \cdots + b_kx_{ik} + e_{ij}, i = 1, 2, ...; j = 1, 2, ..., n_i$ where there are n_j measurements for $(x_{i1}, x_{i2}, ..., x_{ik})$. The random variable y_{ij} is the j-th measurement obtained with $(x_1, x_2, ..., x_k) = (x_{i1}, x_{i2}, ..., x_{ik})$. We need $n_i > 1$ for some i. The parameters δ_i are the lack-of-fit parameters. The test for adequacy of the model is $H_0 : \delta_i = 0, \forall i$ (i.e. the regression model is adequate). The sum of squares for testing H_0 is $Q = SS(E)_{reduced} - SS(E)_{full}$. Now, $SS(E)_{reduced} = \underline{y}^T(I - P_x)\underline{y}$ (since the reduced model is the regular regression model).

$$SS(E)_{full} = \min \sum_{i=1}^{p} \sum_{j=1}^{n_i} (y_{ij} - b_0 - b_1x_{i1} - \cdots - b_kx_{ik} - \delta_i)^2 = \sum_{i=1}^{p} \sum_{j=1}^{n_i} (y_{ij} - \bar{y}_{i\cdot})^2$$

where $\bar{y}_{i\cdot} = \sum_{j=1}^{n_i} \frac{y_{ij}}{n_i}$ which is equal to the SS(pure error). So, $Q = \underline{y}^T(I - P_x)\underline{y}-$ SS(pure error) = SS(lack of fit). The ANOVA table is as follow.

Source	d.f.	SS
Regression (adj)	k	$SS(R)_m$
Error:	$N - k - 1$	$SS(E)$
Lack of fit	$p - k - 1$	$SS(LOF)$
Pure error	$N - p$	$SS(PE)$
Total (adj)	$N - 1$	$SS(T)_{adj}$

p is equal to the number of groups with constant $x's$. Reject $H_0 : \delta_i = 0, \forall i$ iff

$$F = \frac{SS(LOF)/(p - k - 1)}{SS(PE)/(N - p)} > F_\alpha(p - k - 1, N - p).$$

15.15 Confidence Intervals

This section covers pages 107-109 in the text book. Consider estimating $\underline{q}^T\underline{b}$ where $\underline{q}^T = (q_0\ q_1\ \cdots\ q_k)$ is a given vector of constants. We know that the B.L.U.E., G.L.S.E., and under normality, the MLE of $\underline{q}^T\underline{b}$ is $\underline{q}^T\underline{b} = \underline{q}^T(X^TV^{-1}X)^{-1}X^TV^{-1}\underline{y}$. Here, we specialize to $\underline{e} \sim N(\underline{0}, \sigma^2I)$. So $V = \sigma^2I$ and so, $\underline{q}^T\widehat{\underline{b}} = \underline{q}^T(X^TX)^{-1}X^T\underline{y} \Rightarrow \underline{q}^T\widehat{\underline{b}} \sim N(\underline{q}^T\underline{b}, \sigma^2\underline{q}^T(X^TX)^{-1}\underline{q}) \Rightarrow$

$$\frac{\underline{q}^T\widehat{\underline{b}} - \underline{q}^T\underline{b}}{\sigma\sqrt{\underline{q}^T(X^TX)^{-1}\underline{q}}} \sim N(0, 1).$$

Our estimate of σ^2 is $\frac{SS(E)}{N-r(X)}$ where the distribution is $\frac{SS(E)}{N-r(X)} \sim \frac{\sigma^2\chi^2[N-r(X)]}{N-r(X)}$ where $SS(E) = \underline{y}^T(I-P_x)\underline{y}$. Now, $\underline{q}^T\widehat{\underline{b}} = \underline{q}^T(X^TX)^{-1}X^T\underline{y}$ and $SS(E) = \underline{y}^T(I - P_x)\underline{y}$ are independent since by Theorem 2.5 $BVA = \underline{q}^T(X^TX)^{-1}X^T\sigma^2I(I - P_x) = 0$ implies that the chi-square is independent of the $N(0, 1)$. This implies that

$$\frac{\underline{q}^T\widehat{\underline{b}} - \underline{q}\underline{b}}{\sigma\sqrt{\underline{q}^T(X^TX)^{-1}\underline{q}}} \Bigg/ \sqrt{\frac{SS(E)}{\sigma^2(N - r(X))}} \sim t(N - r(X))$$

Hence,

$$P\left(-t_{\alpha/2}(N-r(X)) \le \frac{\underline{q}^T\widehat{\underline{b}} - \underline{q}\underline{b}}{\sqrt{\underline{q}^T(X^TX)^{-1}\underline{q}}\sqrt{MS(E)}} \le t_{\alpha/2}(N-r(X))\right) = 1-\alpha$$

or equivalently

$$P\left[\underline{q}^T\widehat{\underline{b}} - t_{\alpha/2}(N-r(X))SE(\underline{q}^T\widehat{\underline{b}}) \ \le\ \underline{q}^T\underline{b} \ \le\ \underline{q}^T\widehat{\underline{b}} + t_{\alpha/2}(N-r(X))SE(\underline{q}^T\widehat{\underline{b}})\right] = 1-\alpha$$

where $SE(\underline{q}^T\widehat{\underline{b}}) = \sqrt{\underline{q}^T(X^TX)^{-1}\underline{q}}\sqrt{MS(E)}$. So, the $(1-\alpha)100\%$ confidence interval for $\underline{q}^T\underline{b}$ is $\underline{q}^T\widehat{\underline{b}} \pm t_{\alpha/2}(N-r(X))SE(\underline{q}^T\widehat{\underline{b}})$. Note: We can choose $\underline{q}$ to estimate any particular b_i. $\underline{q}^T = (0\ 0\ 0\cdots 1\ \ \cdots 0) \Rightarrow \underline{q}^T\widehat{\underline{b}} = \widehat{b}_i$, $\underline{q}^T(X^TX)^{-1}\underline{q}$ is the $(i+1)$st diagonal element of $(X^TX)^{-1}$. Let $\underline{x}_0^T = (1\ x_{01}\ x_{02}\ \cdots\ x_{0k})$ be a subset of values for the independent variables for which we wish to estimate the response. Let y_0 be the response at this set of x's. Then, $E(y_0) = \underline{x}_0^T\underline{b} \Rightarrow \widehat{y}_0 = \underline{x}_0^T\widehat{\underline{b}}$ is the estimated average response at $\underline{x}_0$. The confidence interval is $\widehat{y}_0 \pm t_{\alpha/2}(N-r(x))\widehat{\sigma}\sqrt{\underline{x}_0^T(X^TX)^{-1}\underline{x}_o}$. Note: To estimate y_0, a new measurement, at $\underline{x} = \underline{x}_0$, instead of $E(y_0)$, the interval is $\widehat{y}_0 \pm t_{\alpha/2}(N-r(x))\widehat{\sigma}\sqrt{1+\underline{x}_0^T(X^TX)^{-1}\underline{x}_o}$.

15.15.1 SAS

SAS provides two main procedures for linear models — PROC REG and PROC GLM. PROC REG is specifically for regression models i.e. cases of linear models for which the X matrix has full column rank. PROC GLM is more general. It can fit linear models whether or not X has full column rank. Aside from the fundamental difference, each procedure has some options that the other does not. In terms of what we have been studying so far in STAT 627 through Chapter 3 of the text book, there are 3 key differences.

1. PROC REG has a very general TEST statement that will let you test any hypothesis of the form $K'\underline{b} = \underline{m}$. The corresponding CONTRAST statement in PROC GLM can only test hypotheses of the form $K'\underline{b} = \underline{0}$. The ESTIMATE statement in PROC GLM also tests $K'\underline{b} = \underline{0}$, but only for K' having just one row.

2. It is difficult to obtain estimates of linear functions $\underline{q}'\underline{b}$ in PROC REG, and unless you are willing to create new variables in the DATA step, is only possible if the first element of $\underline{q}'$ (corresponding to the intercept) is 1. In PROC GLM, there is an ESTIMATE statement which lets you estimate any $\underline{q}'\underline{b}$.

3. PROC REG has a RESTRICT statement that lets you specify a full model and then impose restrictions on $K'\underline{b} = \underline{m}$. PROC GLM has no corresponding capability.

The data we use here illustrate some of these options. It comes from the text book by Rosner (4th edition, 1995). Blood pressure was measured on infants ages 3 to 5 days. Their birth weights were also recorded.

```
data rost1176;
input bweight age bp;
wtage = bweight * age;
label bweight = "birth weight in ounces"
      age     = "current age in days"
  bp      = "systolic blood pressure - mm Hg"
  wtage   = "interaction of bweight and age";
cards;
135 3 89
120 4 90
100 3 83
105 2 77
130 4 92
125 5 98
125 2 82
105 3 85
120 5 96
90 4 95
120 2 80
95 3 79
120 3 86
150 4 97
160 3 92
125 3 88
100 3 .
100 5 .
;
```

```
/*********************************************************************************
The first examples show how to estimate several linear functions with each PROC. We
estimate

a) The average bp for a 3-day old with birth weight = 100.
b) The average bp for a 5-day old with birth weight = 100.
c) the difference in average bp for two such children.

The estimates for (a) and (b) can be done in PROC REG by putting the q' vectors in
the data set with a missing y, then asking for predicted values with the P option and
confidence intervals with the CLM and CLI options. All three are done in PROC GLM
with the estimate statement.
*********************************************************************************/

proc reg;
  model bp = bweight age wtage/p clm cli;
  title "Estimating Linear Functions of b with PROC REG";
run;

proc glm;
  model bp = bweight age wtage;
  estimate "bweight 100 age 3" intercept 1 bweight 100 age 3 wtage 300;
  estimate "bweight 100 age 5" intercept 1 bweight 100 age 5 wtage 500;
  estimate "3-5 diff, bwgt 100" intercept 0 bweight 0 age 2 wtage 200;
  title "Estimating Linear Functions of b with PROC GLM";
run;



/**********************************************************************************
Next, let's test some hypotheses. Here are six different null hypotheses.

a) The average bp for a 3-day old with birih weight = 100 is 75.
b) The average bp for a 5-day old with birth weight = 100 is 100.
c) (a) and (b) are both true.
d) The difference in bp for a 3-day old and a 5-day old, both of birth weight 100 is zero.
e) The difference in bp for a 3-day old and a 5-day old, both of birth weight 100 is 20.
f) The variables bweight and wtage should be removed from the model.

In PROC REG, we use the TEST statement for each hypothesis. In PROC GLM, we use the
CONTRAST statement, but we can not test (a), (b), (c), or (e) in PROC GLM because m is
not zero for any of these hypotheses. Notice that test (d) also appears in the PROC GLM
listing for the example above using the ESTIMATE statement.
*********************************************************************************/

proc reg;
  model bp = bweight age wtage;
  testa: test intercept + 100 * bweight + 3 * age + 300 * wtage = 75;
  testb: test intercept + 100 * bweight + 5 * age + 500 * wtage = 100;
  testc: test intercept + 100 * bweight + 3 * age + 300 * wtage = 75,
              intercept + 100 * bweight + 5 * age + 500 * wtage = 75;
  testd: test 2 * age + 200 * wtage = 0;
  teste: test 2 * age + 200 * wtage = 20;
  testf: test bweight = 0, wtage = 0;
  title "Estimating Linear Functions of b with PROC REG";
run;

proc glm;
  model bp = bweight age wtage;
  contrast 'test (d)' age 2 wtage 200;
  contrast 'test (f)' bweight 1, wtage 1;
  title "Estimating Linear Functions of b with PROC GLM";
run;



/**********************************************************************************
Finally, let's look at two different restricted models.

1) The model corresponding to the restriction in test (e).
2) The model corresponding to the restriction in test (f).

Restricted models are easily fit in PROC REG with the RESTRICT statement. The restriction
is specified as one or more linear functions, just like in the TEST statement. Alternatively,
you can fit a restricted model by reparametrizing. Both methods are shown below. The
reparameterization model for model 1 requires creating a new variable in the data set. For
model 2, just leave bweight and wtage out of the MODEL statement.

*********************************************************************************/

proc reg;
  model bp = bweight age wtage;
  restrict 2 * age + 200 * wtage = 20;
  title "Fitting Model 1 by Using the RESTRICT Statement";
  title2 "Dr Morgan Suspects SAS has a Bug with the RESTRICT Statement Since the Sums of Squares Don't Match the Reparameterized Model";
run;

data new;
set rost1176;
  bpstar = bp - 0.10 * wtage;
  agestar = age - 0.10 * wtage;
run;

proc reg;
  model bpstar = bweight agestar;
  title "Fitting Model 1 by Reparameterizing";
  title2 "Dr Morgan Suspects SAS has a Bug with the RESTRICT Statement Since the Sums of Squares Don't Match the Reparameterized Model";
run;

proc reg;
  model bp = bweight age wtage;
  restrict bweight = 0, wtage = 0;
  title "Fitting Model 2 by Using the RESTRICT Statement";
  title2 "Dr Morgan says these Sums of Squares Match Because m = 0";
run;
```

```
proc reg;
  model bp = age;
  title "Fitting Model 2 by Reparameterizing";
run;
```

```
                           Estimating Linear Functions of b with PROC REG                          86
                                                                         14:09 Sunday, August 31, 2008

                                         The REG Procedure
                                           Model: MODEL1
                       Dependent Variable: bp systolic blood pressure - mm Hg

                       Number of Observations Read                       18
                       Number of Observations Used                       16
                       Number of Observations with Missing Values         2


                                        Analysis of Variance

                                               Sum of           Mean
            Source                   DF       Squares         Square    F Value    Pr > F

            Model                     3     618.18331      206.06110      46.87    <.0001
            Error                    12      52.75419        4.39618
            Corrected Total          15     670.93750


                        Root MSE              2.09671    R-Square     0.9214
                        Dependent Mean       88.06250    Adj R-Sq     0.9017
                        Coeff Var             2.38093


                                        Parameter Estimates

                                                          Parameter       Standard
Variable     Label                             DF          Estimate          Error    t Value    Pr > |t|

Intercept    Intercept                          1           2.55158       20.83776       0.12      0.9046
bweight      birth weight in ounces             1           0.55123        0.17373       3.17      0.0080
age          current age in days                1          21.28730        6.22363       3.42      0.0051
wtage        interaction of bweight and age     1          -0.12821        0.05159      -2.49      0.0287

                           Estimating Linear Functions of b with PROC REG                          87
                                                                         14:09 Sunday, August 31, 2008

                                         The REG Procedure
                                           Model: MODEL1
                       Dependent Variable: bp systolic blood pressure - mm Hg

                                         Output Statistics

           Dependent  Predicted     Std Error
      Obs   Variable      Value  Mean Predict       95% CL Mean        95% CL Predict      Residual

        1    89.0000    88.9055        0.7869    87.1910    90.6200    84.0260    93.7849    0.0945
        2    90.0000    92.3086        0.6642    90.8615    93.7558    87.5166    97.1007   -2.3086
        3    83.0000    83.0742        0.8308    81.2641    84.8843    78.1604    87.9881   -0.0742
        4    77.0000    76.0819        1.3601    73.1184    79.0453    70.6365    81.5272    0.9181
        5    92.0000    92.6926        0.7428    91.0743    94.3110    87.8461    97.5391   -0.6926
        6    98.0000    97.7619        1.1479    95.2609   100.2629    92.5537   102.9700    0.2381
        7    82.0000    81.9782        1.0322    79.7292    84.2272    76.8863    87.0701    0.0218
        8    85.0000    83.9073        0.7160    82.3472    85.4673    79.0799    88.7346    1.0927
        9    96.0000    98.2109        1.1088    95.7951   100.6268    93.0431   103.3787   -2.2109
       10    95.0000    91.1567        1.6120    87.6444    94.6689    85.3942    96.9191    3.8433
       11    80.0000    80.5041        0.9222    78.4947    82.5135    75.5134    85.4948   -0.5041
       12    79.0000    82.2412        0.9610    80.1474    84.3349    77.2159    87.2665   -3.2412
       13    86.0000    86.4064        0.5611    85.1838    87.6290    81.6773    91.1355   -0.4064
       14    97.0000    93.4606        1.4203    90.3661    96.5552    87.9428    98.9784    3.5394
       15    92.0000    93.0707        1.4974    89.8081    96.3332    87.4569    98.6844   -1.0707
       16    88.0000    87.2394        0.6004    85.9312    88.5476    82.4874    91.9914    0.7606
       17          .    83.0742        0.8308    81.2641    84.8843    78.1604    87.9881          .
       18          .   100.0071        2.2483    95.1086   104.9056    93.3090   106.7053          .


                            Sum of Residuals                         0
                            Sum of Squared Residuals          52.75419
                            Predicted Residual SS (PRESS)    174.81661

                           Estimating Linear Functions of b with PROC GLM                          88
                                                                         14:09 Sunday, August 31, 2008

                                         The GLM Procedure

                              Number of Observations Read          18
                              Number of Observations Used          16

                           Estimating Linear Functions of b with PROC GLM                          89
                                                                         14:09 Sunday, August 31, 2008

                                         The GLM Procedure

Dependent Variable: bp   systolic blood pressure - mm Hg

                                                 Sum of
         Source                      DF         Squares     Mean Square    F Value    Pr > F

         Model                        3     618.1833074     206.0611025      46.87    <.0001

         Error                       12      52.7541926       4.3961827

         Corrected Total             15     670.9375000


                         R-Square     Coeff Var      Root MSE       bp Mean

                         0.921372      2.380931      2.096708      88.06250
```

```
Source                     DF       Type I SS     Mean Square    F Value    Pr > F

bweight                     1     130.5375000     130.5375000      29.69    0.0001
age                         1     460.4981398     460.4981398     104.75    <.0001
wtage                       1      27.1476676      27.1476676       6.18    0.0287


Source                     DF     Type III SS     Mean Square    F Value    Pr > F

bweight                     1     44.25798931     44.25798931      10.07    0.0080
age                         1     51.43153031     51.43153031      11.70    0.0051
wtage                       1     27.14766758     27.14766758       6.18    0.0287


                                                 Standard
    Parameter                  Estimate           Error    t Value    Pr > |t|

    bweight 100 age 3         83.074216      0.83075825     100.00      <.0001
    bweight 100 age 5        100.007106      2.24825226      44.48      <.0001
    3-5 diff, bwgt 100        16.932890      2.37299834       7.14      <.0001


                                            Standard
         Parameter         Estimate           Error    t Value    Pr > |t|

         Intercept       2.55158089     20.83776184       0.12      0.9046
         bweight         0.55123300      0.17373097       3.17      0.0080
         age            21.28729601      6.22362825       3.42      0.0051
         wtage          -0.12820851      0.05159272      -2.49      0.0287

                   Estimating Linear Functions of b with PROC REG                            90
                                                              14:09 Sunday, August 31, 2008

                                 The REG Procedure
                                   Model: MODEL1
               Dependent Variable: bp systolic blood pressure - mm Hg

               Number of Observations Read                      18
               Number of Observations Used                      16
               Number of Observations with Missing Values        2


                                Analysis of Variance

                                       Sum of           Mean
  Source                   DF         Squares         Square    F Value    Pr > F

  Model                     3       618.18331      206.06110      46.87    <.0001
  Error                    12        52.75419        4.39618
  Corrected Total          15       670.93750


               Root MSE              2.09671    R-Square     0.9214
               Dependent Mean       88.06250    Adj R-Sq     0.9017
               Coeff Var             2.38093


                                Parameter Estimates

                                                  Parameter       Standard
Variable     Label                          DF     Estimate          Error    t Value    Pr > |t|

Intercept    Intercept                       1      2.55158       20.83776       0.12      0.9046
bweight      birth weight in ounces          1      0.55123        0.17373       3.17      0.0080
age          current age in days             1     21.28730        6.22363       3.42      0.0051
wtage        interaction of bweight and age  1     -0.12821        0.05159      -2.49      0.0287

                   Estimating Linear Functions of b with PROC REG                            91
                                                              14:09 Sunday, August 31, 2008

                                 The REG Procedure
                                   Model: MODEL1

                   Test testa Results for Dependent Variable bp

                                             Mean
             Source            DF          Square    F Value    Pr > F

             Numerator          1       415.26672      94.46    <.0001
             Denominator       12         4.39618

                   Estimating Linear Functions of b with PROC REG                            92
                                                              14:09 Sunday, August 31, 2008

                                 The REG Procedure
                                   Model: MODEL1

                   Test testb Results for Dependent Variable bp

                                             Mean
             Source            DF          Square    F Value    Pr > F

             Numerator          1      0.00004391       0.00    0.9975
             Denominator       12         4.39618

                   Estimating Linear Functions of b with PROC REG                            93
                                                              14:09 Sunday, August 31, 2008

                                 The REG Procedure
                                   Model: MODEL1

                   Test testc Results for Dependent Variable bp

                                             Mean
             Source            DF          Square    F Value    Pr > F
```

```
                Numerator           2      465.54799     105.90    <.0001
                Denominator        12        4.39618

                     Estimating Linear Functions of b with PROC REG                            94
                                                                        14:09 Sunday, August 31, 2008

                                   The REG Procedure
                                     Model: MODEL1

                     Test testd Results for Dependent Variable bp

                                                   Mean
                Source             DF            Square    F Value    Pr > F

                Numerator           1      223.84275      50.92    <.0001
                Denominator        12        4.39618

                     Estimating Linear Functions of b with PROC REG                            95
                                                                        14:09 Sunday, August 31, 2008

                                   The REG Procedure
                                     Model: MODEL1

                     Test teste Results for Dependent Variable bp

                                                   Mean
                Source             DF            Square    F Value    Pr > F

                Numerator           1        7.34412       1.67    0.2205
                Denominator        12        4.39618

                     Estimating Linear Functions of b with PROC REG                            96
                                                                        14:09 Sunday, August 31, 2008

                                   The REG Procedure
                                     Model: MODEL1

                     Test testf Results for Dependent Variable bp

                                                   Mean
                Source             DF            Square    F Value    Pr > F

                Numerator           2       54.68337      12.44    0.0012
                Denominator        12        4.39618

                     Estimating Linear Functions of b with PROC GLM                            97
                                                                        14:09 Sunday, August 31, 2008

                                   The GLM Procedure

                        Number of Observations Read          18
                        Number of Observations Used          16

                     Estimating Linear Functions of b with PROC GLM                            98
                                                                        14:09 Sunday, August 31, 2008

                                   The GLM Procedure

Dependent Variable: bp   systolic blood pressure - mm Hg

                                              Sum of
         Source                    DF         Squares     Mean Square    F Value    Pr > F

         Model                      3     618.1833074     206.0611025      46.87    <.0001

         Error                     12      52.7541926       4.3961827

         Corrected Total           15     670.9375000


                  R-Square     Coeff Var      Root MSE       bp Mean

                  0.921372      2.380931      2.096708      88.06250


         Source                    DF       Type I SS     Mean Square    F Value    Pr > F

         bweight                    1     130.5375000     130.5375000      29.69    0.0001
         age                        1     460.4981398     460.4981398     104.75    <.0001
         wtage                      1      27.1476676      27.1476676       6.18    0.0287


         Source                    DF     Type III SS     Mean Square    F Value    Pr > F

         bweight                    1     44.25798931     44.25798931      10.07    0.0080
         age                        1     51.43153031     51.43153031      11.70    0.0051
         wtage                      1     27.14766758     27.14766758       6.18    0.0287


         Contrast                  DF     Contrast SS     Mean Square    F Value    Pr > F

         test (d)                   1     223.8427463     223.8427463      50.92    <.0001
         test (f)                   2     109.3667376      54.6833688      12.44    0.0012


                                                 Standard
              Parameter         Estimate            Error    t Value    Pr > |t|

              Intercept       2.55158089      20.83776184       0.12      0.9046
              bweight         0.55123300       0.17373097       3.17      0.0080
              age            21.28729601       6.22362825       3.42      0.0051
              wtage          -0.12820851       0.05159272      -2.49      0.0287

                       Fitting Model 1 by Using the RESTRICT Statement                         99
Dr Morgan Suspects SAS has a Bug with the RESTRICT Statement Since the Sums of Squares Don't Match the
                                                                        14:09 Sunday, August 31, 2008
```

```
                                    The REG Procedure
                                      Model: MODEL1
                    Dependent Variable: bp systolic blood pressure - mm Hg

NOTE: Restrictions have been applied to parameter estimates.


                    Number of Observations Read                        18
                    Number of Observations Used                        16
                    Number of Observations with Missing Values          2


                                   Analysis of Variance

                                          Sum of           Mean
            Source                 DF        Squares         Square    F Value    Pr > F

            Model                   2      610.83919      305.41959      66.07    <.0001
            Error                  13       60.09831        4.62295
            Corrected Total        15      670.93750


                     Root MSE              2.15010    R-Square     0.9104
                     Dependent Mean       88.06250    Adj R-Sq     0.8966
                     Coeff Var             2.44157


                                   Parameter Estimates

                                                 Parameter       Standard
Variable     Label                         DF      Estimate          Error    t Value    Pr > |t|

Intercept    Intercept                      1     -21.56230        9.51748      -2.27      0.0412
bweight      birth weight in ounces         1       0.74292        0.09280       8.01      <.0001
age          current age in days            1      28.65302        2.56516      11.17      <.0001
wtage        interaction of bweight and age 1      -0.18653        0.02565      -7.27      <.0001
RESTRICT                                   -1      -2.39447        1.89977      -1.26      0.2205*

                       * Probability computed using beta distribution.

                              Fitting Model 1 by Reparameterizing                            100
Dr Morgan Suspects SAS has a Bug with the RESTRICT Statement Since the Sums of Squares Don't Match the
                                                               14:09 Sunday, August 31, 2008

                                    The REG Procedure
                                      Model: MODEL1
                                Dependent Variable: bpstar

                    Number of Observations Read                        18
                    Number of Observations Used                        16
                    Number of Observations with Missing Values          2


                                   Analysis of Variance

                                          Sum of           Mean
            Source                 DF        Squares         Square    F Value    Pr > F

            Model                   2      837.77980      418.88990      53.67    <.0001
            Error                  13      101.45457        7.80420
            Corrected Total        15      939.23438


                     Root MSE              2.79360    R-Square     0.8920
                     Dependent Mean       48.03125    Adj R-Sq     0.8754
                     Coeff Var             5.81621


                                   Parameter Estimates

                                             Parameter       Standard
    Variable     Label                   DF      Estimate          Error    t Value    Pr > |t|

    Intercept    Intercept                1      70.89053        4.73553      14.97      <.0001
    bweight      birth weight in ounces   1      -0.01493        0.04706      -0.32      0.7561
    agestar                               1       0.57364        0.06925       8.28      <.0001

                       Fitting Model 2 by Using the RESTRICT Statement                       101
                   Dr Morgan says these Sums of Squares Match Because m = 0
                                                               14:09 Sunday, August 31, 2008

                                    The REG Procedure
                                      Model: MODEL1
                    Dependent Variable: bp systolic blood pressure - mm Hg

NOTE: Restrictions have been applied to parameter estimates.


                    Number of Observations Read                        18
                    Number of Observations Used                        16
                    Number of Observations with Missing Values          2


                                   Analysis of Variance

                                          Sum of           Mean
            Source                 DF        Squares         Square    F Value    Pr > F

            Model                   1      508.81657      508.81657      43.94    <.0001
            Error                  14      162.12093       11.58007
            Corrected Total        15      670.93750


                     Root MSE              3.40295    R-Square     0.7584
                     Dependent Mean       88.06250    Adj R-Sq     0.7411
                     Coeff Var             3.86424
```

Parameter Estimates

Variable	Label	DF	Parameter Estimate	Standard Error	t Value	Pr > |t|
Intercept	Intercept	1	67.67907	3.19056	21.21	<.0001
bweight	birth weight in ounces	1	8.89393E-17	0	Infty	<.0001
age	current age in days	1	6.15349	0.92832	6.63	<.0001
wtage	interaction of bweight and age	1	-1.4152E-17	0	-Infty	<.0001
RESTRICT		-1	654.69767	245.70276	2.66	0.0029*
RESTRICT		-1	1961.83721	827.36819	2.37	0.0112*

* Probability computed using beta distribution.

Fitting Model 2 by Reparameterizing 102
14:09 Sunday, August 31, 2008

The REG Procedure
Model: MODEL1
Dependent Variable: bp systolic blood pressure - mm Hg

Number of Observations Read	18
Number of Observations Used	16
Number of Observations with Missing Values	2

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	1	508.81657	508.81657	43.94	<.0001
Error	14	162.12093	11.58007		
Corrected Total	15	670.93750			

Root MSE	3.40295	R-Square	0.7584
Dependent Mean	88.06250	Adj R-Sq	0.7411
Coeff Var	3.86424		

Parameter Estimates

Variable	Label	DF	Parameter Estimate	Standard Error	t Value	Pr > |t|
Intercept	Intercept	1	67.67907	3.19056	21.21	<.0001
age	current age in days	1	6.15349	0.92832	6.63	<.000

15.16 Models Not of Full Rank

We still have the linear model $\underline{y}_{N\times 1} = X_{N\times p}\ \underline{b}_{p\times 1} + \underline{e}_{N\times 1}$, where $E(\underline{e}) = 0$ and $Var(\underline{e}) = V$ is positive definite. But, no longer is the rank $r(X)$ equal to the number of columns in X. If we want to find the generalized least squares estimates, we minimize $(\underline{y} - X\underline{b})^T V^{-1}(\underline{y} - X\underline{b})$ with respect to $\underline{b}$ giving the normal equations $(X^TV^{-1}X)\underline{b} = X^TV^{-1}\underline{y}$. The rank $r(X^TV^{-1}X) = r(X)$ may not be p. It may be less than p. Noting that the equations are consistent, a solution is $\underline{b}^0 = (X^TV^{-1}X)^- X^TV^{-1}\underline{y} = GX^TV^{-1}\underline{y}$ where G is any g-inverse of $(X^TV^{-1}X)$. Of course there are many such solutions. So we can not say that $\underline{b}^0$ is an estimate of $\underline{b}$. Hence we ask, "what can we estimate?" To answer the question, we introduce the concept of an estimable function. A linear function $\underline{q}^T\underline{b}$ of the vector of parameters $\underline{b}$ is said to be *linearly estimable* if there is a linear function of the y's with the expected value $\underline{q}^T\underline{b}$. So, $\underline{q}^T\underline{b}$ is estimable iff $\exists \underline{t} \ni$: $E(\underline{t}^T\underline{y}) = \underline{q}^T\underline{b}$ iff $\exists \underline{t} \ni$: $\underline{t}^TX\underline{b} = \underline{q}^T\underline{b}, \forall \underline{b}$ iff $\exists \underline{t} \ni$: $\underline{t}^TX = \underline{q}^T$ iff $\underline{q}^T \in \Re(X)$. Since $\Re(X) = \Re(X^TV^{-1}X)$, we can write $\underline{q}^T = \underline{t}^TX = \underline{s}^TX^TV^{-1}X$, for some $\underline{t}$ and $\underline{s}$. Now, for $\underline{b}^0$. Any solution of $E(\underline{q}^T\underline{b}^0) = \underline{q}^TE(\underline{b}^0) = \underline{q}^TE(GX^TV^{-1}\underline{y}) = \underline{q}^TGX^TV^{-1}X\underline{b} = \underline{s}^TX^TV^{-1}XGX^TV^{-1}X\underline{b} = \underline{s}^T(X^TV^{-1}X)\underline{b} = \underline{q}^t\underline{b}$, i.e. if $\underline{q}^T\underline{b}$ is estimable, then $\underline{q}^T\underline{b}^0$ is an unbiased estimator of $\underline{q}^T\underline{b}$. What is the variance of $\underline{q}^T\underline{b}^0$? $Var(\underline{q}^T\underline{b}^0) = \underline{q}^TVar(\underline{b}^0)\underline{q} = \underline{q}^TVar(GX^TV^{-1}\underline{y})\underline{q} = \underline{q}^TGX^TV^{-1}VV^{-1}XG^T\underline{q} = \underline{q}^TG(X^TV^{-1}X)G^T\underline{q} = \underline{q}^TG\overbrace{(X^TV^{-1}X)G^T(X^TV^{-1}X)}^{X^TV^{-1}X}\underline{s} = \underline{q}^TG(X^TV^{-1}X)\underline{s} = \underline{q}^TG\underline{q}$. We now show that $\underline{q}^T\underline{b}^0$ is the B.L.U.E. of $\underline{q}^T\underline{b}$. Let $\underline{k}^T\underline{y}$ be any other unbiased estimator of $\underline{q}^T\underline{b}$. Then, $E(\underline{k}^T\underline{y}) = \underline{k}^TX\underline{b} = \underline{q}^T\underline{b}, \forall\underline{b} \Rightarrow \underline{k}^TX = \underline{q}^T.0 \leq Var(\underline{q}^T\underline{b}^0 - \underline{k}^T\underline{y}) = Var(\underline{q}^T\underline{b}^0) + Var(\underline{k}^T\underline{y}) - 2Cov(\underline{q}^T\underline{b}^0, \underline{k}^T\underline{y}) = \underline{q}^TG\underline{q} + Var(\underline{k}^T\underline{y}) - 2\underline{q}^TCov(\underline{b}^0, \underline{y})\underline{k} = \underline{q}^TG\underline{q} + Var(\underline{k}^T\underline{y}) - 2\underline{q}^TCov(GX^TV^{-1}\underline{y}, \underline{y})\underline{k} = \underline{q}^TG\underline{q} + Var(\underline{k}^T\underline{y}) - 2\underline{q}^TGX^TV^{-1}V\underline{k} = \underline{q}^TG\underline{q} + Var(\underline{k}^T\underline{y}) - 2\underline{q}^TG\underline{q} = Var(\underline{k}^T\underline{y}) - \underline{q}^TG\underline{q} = Var(\underline{k}^T\underline{y}) - Var(\underline{q}^T\underline{b}^0) \Rightarrow Var(\underline{k}^T\underline{y}) \geq Var(\underline{q}^T\underline{b}^0)$.

Variances depend on G. Covariances do not depend on G. Note that $Var(\underline{b}^0) = Var(GX^TV^{-1}\underline{y}) =$

$GX^TV^{-1}VV^{-1}XG^T = G(X^TV^{-1}X)G^T$ depends on G. If $\underline{q}^T\underline{b}$ and $\underline{p}^T\underline{b}$ are both estimable, then the

$Cov(\underline{q}^T\underline{b}^0, \underline{p}^T\underline{b}^0) = \underline{q}^TCov(\underline{b}^0, \underline{b}^0)\underline{p} = \underline{q}^TG(X^TV^{-1}X)G^T\underline{p} = \underline{q}^TG\overbrace{(X^TV^{-1}X)G^T(X^TV^{-1}X)}^{X^TV^{-1}X}\underline{w} = \underline{q}^TG\underline{p}$ does not depend on G where $\underline{p}^T = \underline{w}^TX^TV^{-1}X$

Theorem 5.1: Consider the linear model $\underline{y} = X\underline{b} + \underline{e}$, $E(\underline{e}) = 0$ and $Var(\underline{e}) = V$ is positive definite. X does not have full column rank. Let $\underline{b}^0$ be any solution to the normal equations $(X^TV^{-1}X)\underline{b} = X^TV^{-1}\underline{y}$. That is, $\underline{b}^0 = GX^TV^{-1}\underline{y}$ where G is any g-inverse of $(X^TV^{-1}X)$. Then,

1. Although $\underline{b}^0$ is in no sense an estimate of $\underline{b}$, $\underline{q}^T\underline{b}^0$ is the B.L.U.E. of $\underline{q}^T\underline{b}$ for any $\underline{q}^T \in \Re(X)$.
2. Although G is not, in general, the variance of $\underline{b}^0$, $Cov(\underline{q}^T\underline{b}^0, \underline{p}^T\underline{b}^0) = \underline{q}^TG\underline{p}$ for any $\underline{q}^T$, $\underline{p}^T \in \Re(X)$. In particular, $Var(\underline{q}^T\underline{b}^0) = \underline{q}^TG\underline{q}$. A special case of this is $V = \sigma^2I$.

Corollary 5.1: Let $\underline{y} = X\underline{b} + \underline{e}$, where $E(\underline{e}) = 0$ and $Var(\underline{e}) = \sigma^2I$ and X does not have full column rank. (Remember, when X does not have full column rank, use G for $(X^TX)^{-1}$ and only estimate estimable functions. Otherwise do everything the same way). Let $\underline{b}^0$ be any solutions to the normal equations $X^TX\underline{b} = X^T\underline{y}$, i.e. $\underline{b}^0 = GX^T\underline{y}$ where G is any g-inverse of X^TX. Then,

1. $\underline{q}^T\underline{b}^0$ is the B.L.U.E. of $\underline{b}$ for any $\underline{q}^T \in \Re(X)$.
2. $Cov(\underline{q}^T\underline{b}^0, \underline{p}^T\underline{b}^0) = \underline{q}^TG\underline{p}$ for any $\underline{q}^T$, $\underline{p}^T \in \Re(X)$.

Other facts about estimability include.

1. There are $r(X)$ linearly independent estimable functions.
2. $\underline{q}^T\underline{b}$ is estimable iff $\underline{q}^TH = \underline{q}^T$ where $H = (X^TV^{-1}X)^-(X^TV^{-1}X)$. For $V = \sigma^2I$, this is $H = (X^TX)^-(X^TX)$.

Example: This is the six rubber plants example on page 166 of the text book. X^TX has rank $r(X) = 3$.

$$X^TX = \begin{pmatrix} 6 & 3 & 2 & 1 \\ 3 & 3 & 0 & 0 \\ 2 & 0 & 2 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \quad G_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad G_2 = \begin{pmatrix} 1 & -1 & -1 & 0 \\ -1 & \frac{4}{3} & 1 & 0 \\ -1 & 1 & \frac{3}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

G_1 and G_2 are each g-inverses of X^TX. Suppose $\underline{y}^T = (101\ \ 105\ \ 94\ \ 84\ \ 88\ \ 321)$. $X^T\underline{y} = (504\ \ 300\ \ 172\ \ 32)^T$.

$$G_1X^T\underline{y} = \begin{pmatrix} 0 \\ 100 \\ 86 \\ 32 \end{pmatrix} = \underline{b}_1, \;\; G_2X^T\underline{y} = \begin{pmatrix} 32 \\ 68 \\ 54 \\ 0 \end{pmatrix} = \underline{b}_2 \;\; H = G_1(X^TX) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}.$$

We can estimate any $\underline{q}^T\underline{b}$ which $\underline{q}^TH = \underline{q}^T$. Consider $\underline{q}^T = (0\ 1\ 0\ 0)$ so that $\underline{q}^T\underline{b} = \alpha_1$. Note that $\underline{q}^TH = (1\ 1\ 0\ 0) \neq \underline{q}^T$. This implies that $\underline{q}^T$ is not an estimable function. Also, $\underline{q}^T\underline{b}_1 = 100 \neq 68 = \underline{q}^T\underline{b}_2$ which is further evidence that this is not an estimable function. Consider $\underline{q}^T = (0\ 1\ -1\ 0)$ so that $\underline{q}^T\underline{b} = \alpha_1 - \alpha_2$. Now, $\underline{q}^TH = (0\ 1\ -1\ 0) = \underline{q}^T$. Then, $\alpha_1 - \alpha_2$ is an estimable function. $\underline{q}^T\underline{b}_1 = 100 - 86 = 14$ and $\underline{q}^T\underline{b}_2 = 68 - 54 = 14$. This implies that $\underline{q}^T\underline{b}_1 = \underline{q}^T\underline{b}_2$.

Example: This is a continuation of the six rubber plant example above from the text book.

$$X = \begin{array}{c} \begin{array}{cccc} \mu & \alpha_1 & \alpha_2 & \alpha_3 \end{array} \\ \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix} \end{array}, \quad \underline{y} = \begin{pmatrix} 101 \\ 105 \\ 94 \\ 84 \\ 88 \\ 32 \end{pmatrix}, \quad X^T\underline{y} = \begin{pmatrix} 504 \\ 300 \\ 172 \\ 32 \end{pmatrix}, \quad G = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

$$\underline{b}^0 = GX^T\underline{y} = \begin{pmatrix} 0 \\ 100 \\ 86 \\ 32 \end{pmatrix}.$$

$SS(T) = \underline{y}^T\underline{y} = (101)^2 + \cdots + (32)^2 = 45886.$

$$SS(R) = \underline{y}^T P_X \underline{y} = \underline{y}^T X G X^T \underline{y} = \underline{y}^T X \underline{b}^0 = (504,\ \ 300,\ \ 172,\ \ 32) \begin{pmatrix} 0 \\ 100 \\ 86 \\ 32 \end{pmatrix} = 45816.$$

$SS(E) = \underline{y}^T(I - P_X)\underline{y} = \underline{y}^T\underline{y} - \underline{y}^T P_X \underline{y} = SS(T) - SS(R) = 45886 - 45816 = 70$. $SS(M) = \frac{1}{N}\underline{y}^T J \underline{y} = \frac{1}{N}\left(\sum y_i\right)^2 = \frac{1}{6}(504)^2 = 42336$. $SSR(M) = SS(R) - SS(M) = 45816 - 42336 = 3480$.

Source	SS	d.f.	MS	F	p-value
Mean	42336	1	42336	1814.4	0.001
Model (adj for mean)	3480	2	1740	74.57	$0.005 \geq p \geq 0.001$
Error	70	3	23.33		
Total	45886	6			

$H_0 : E(\bar{y}) = 0$, i.e. $H_0 : \mu + \frac{3\alpha_1}{6} + \frac{2\alpha_2}{6} + \frac{\alpha_3}{6} = 0$ or $H_0 : \mu + \frac{\alpha_1}{2} + \frac{\alpha_2}{3} + \frac{\alpha_3}{6} = 0$. $F = 1814.4$. Reject H_0 at $\alpha = 0.001$ level. $H_0 : \mu_1 = \mu_2 = \mu_3 = \mu_4 = \mu_5 = \mu_6$, i.e. $H_0 : \mu + \alpha_1 = \mu + \alpha_1 = \mu + \alpha_1 = \mu + \alpha_2 = \mu + \alpha_2 = \mu + \alpha_3$ or $H_0 : \alpha_1 = \alpha_2 = \alpha_3$. $F = 74.57$ Reject H_0 at $\alpha = 0.005$ level. The ANOVA table for $H_0 : K^T\underline{b} = \underline{0}$ is

Source	d.f.	SS
Full Model	r	$SS(R) = \underline{y}^T P_X \underline{y}$
Hypothesis	s	$Q = \underline{y}^T A_H \underline{y}$
Reduced Model	$r - s$	$SS(R)_{reduced} = \underline{y}^T (P_X - A_H)\underline{y}$
Residual Error	$N - r$	$SS(E) = \underline{y}^T (I - P_X)\underline{y}$
Total	N	$SS(T) = \underline{y}^T \underline{y}$

Alternatively, the ANOVA table for $H_0 : K^T\underline{b} = \underline{0}$ after fitting the mean is

Source	d.f.	SS
Full Model (after mean)	$r - 1$	$SSR(M) = SS(R) - \frac{1}{N}\underline{y}^T J \underline{y}$
Hypothesis	s	Q
Reduced Model (after mean)	$r - s - 1$	$SS(R)_{reduced} - \frac{1}{N}\underline{y}^T J \underline{y}$
Residual Error	$N - r$	$SS(E)$
Total (after mean)	$N - 1$	$SST(M) = SS(T) - \frac{1}{N}\underline{y}^T J \underline{y}$

This ANOVA table holds true provided that $\underline{j}^T X \notin \Re(K^T)$ i.e. $K^T\underline{b} = \underline{0}$ does not include $\underline{j}^T X \underline{b} = \underline{0}$, which is the hypothesis tested by $SS(M)$.

Example: This is a continuation of the 6 rubber plants example in this section. Consider the hypothesis $H_0 : \alpha_1 = \alpha_2$. $K^T = (0,\ 1,\ -1,\ 0)$. $m = 0$.

$$K^T \underline{b}^0 = (0,\ 1,\ -1,\ 0) \begin{pmatrix} 0 \\ 100 \\ 86 \\ 32 \end{pmatrix} = 100 - 86 = 14.$$

$$K^T G K = (0,\ 1,\ -1,\ 0) \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = \frac{1}{3} + \frac{1}{2} = \frac{5}{6}.$$

$Q = (K^T\underline{b}^0)^T (K^T G K)^{-1} (K^T \underline{b}^0) = 14 \left(\frac{5}{6}\right)^{-1} 14 = 235.2$

Source	d.f.	SS	MS	F
Full Model (after mean)	2	3480	74.57	
Hypothesis	1	235.2	235.2	10.08
Reduced Model (after mean)	1	3244.8	3244.8	139.06
Residual Error	3	70	23.33	
Total (after mean)	5	3550		

$F_{0.05}(1,3) = 10.1$ and $F_{0.005}(1,3) = 55$. The reduced model has $\alpha_1 = \alpha_2$ i.e.

$$E(y_i) = \begin{cases} \mu + \alpha_1, & i = 1,2,3,4,5. \\ \mu + \alpha_3, & i = 6. \end{cases}$$

15.17 Test of Hypotheses ($V = \sigma^2 I$)

The general linear hypothesis of order s specifies the value of s ($s \le r(X)$) independent *estimable* linear functions of $\underline{b}$. Hence it may be written $H : K^T\underline{b} = \underline{m}$, where $K^T = S^T X^T X$, and S^T has full row rank and K^T is $s \times p$ of rank $r(S) \le r(X) \le p$. We assume that $\underline{y} = X\underline{b} + \underline{e}$ where $\underline{e} \sim N(\underline{0}, \sigma^2 I)$ and wish to find the likelihood ratio test for H. With the same argument used in the full rank case, the test statistic will be

$$\frac{N - r(X)}{r(K)} \frac{\left\{ \min_{K^T\underline{b}=\underline{m}} \left(\underline{y} - X\underline{b}\right)^T \left(\underline{y} - X\underline{b}\right) - \min\left(\underline{y} - X\underline{b}\right)^T \left(\underline{y} - X\underline{b}\right)\right\}}{\min\left(\underline{y} - X\underline{b}\right)^T \left(\underline{y} - X\underline{b}\right)}$$

where all the min's being with respect to $\underline{b}$. $\min(\underline{y}-X\underline{b})^T(\underline{y}-X\underline{b}) = (\underline{y}-X\underline{b}^0)^T(\underline{y}-X\underline{b}^0) = (\underline{y}-XGX^T\underline{y})^(\underline{y}-XGX^T\underline{y}) = (\underline{y} - P_x\underline{y})^T(\underline{y} - P_x\underline{y}) = \underline{y}^T(I - P_x)^T(I - P_x)\underline{y} = \underline{y}^T(I - P_x)\underline{y} = SS(E)$.

$\min_{K^T\underline{b}=m}(\underline{y} - X\underline{b})^T(\underline{y} - X\underline{b})$ is found as before. Let $2\underline{\theta}$ be a vector of Lagrange multipliers and write $F = (\underline{y}-X\underline{b})^T(\underline{y}-X\underline{b})+2(\underline{b}^T K-\underline{m}^T)\underline{\theta}$. $\frac{1}{2}\frac{dF}{d\underline{b}} = -X^T\underline{y}+X^TX\underline{b}+K\theta = \underline{0} \Rightarrow X^TX\underline{b}^0_H = X^T\underline{y}-K\underline{\theta} \Rightarrow \underline{b}^0_H = GX^T\underline{y}-GK\underline{\theta}$ where G is a g-inverse of $X^TX = \underline{b}^0 - GK\underline{\theta} \Rightarrow GK\underline{\theta} = \underline{b}^0 - \underline{b}^0_H$. $K^TGK\underline{\theta} = K^T(\underline{b}^0 - \underline{b}^0_H)$. Now, $K^T\underline{b}$ is estimable which implies that $K^T = S^TX^TX \Rightarrow K^TGK = S^T(X^TX)G(X^TX)S = S^T(X^TX)S = L^TL$ where $L = XS \Rightarrow r(K) \ge r(K^TGK) = r(L^TL) = r(L) = r(XS) \ge r(X^TXS) = r(K) \Rightarrow r(K^TGK) = r(k) = s \Rightarrow K^TGK$ is non-singular which implies that $\underline{\theta} = (K^TGK)^{-1}K^T(\underline{b}^0 - \underline{b}^0_H) \Rightarrow \underline{b}^0_H = \underline{b}_0 - GK(K^TGK)^{-1}K^T(\underline{b}^0 - \underline{b}^0_H) = GX^T\underline{y} - GK(K^TGK)^{-1}K^T(\underline{b}^0 - \underline{b}^0_H)$. Compare that to Chapter 3 in the text book. The rest of the argument goes just as before so that $Q = SS(E)_{red} - SS(E)_{full} = (\underline{y}-X\underline{b}^0_H)^T(\underline{y}-X\underline{b}^0_H)-(\underline{y}-X\underline{b}^0)^T(\underline{y}-X\underline{b}^0) = \cdots = (K^T\underline{b}^0-\underline{m})^T(K^TGK)^{-1}(K^T\underline{b}^0-\underline{m})$. General Rule: Non-centrality always equals $\frac{1}{2\sigma^2}$(Expected value)^T(Quadratic form)(Expected value). Clearly, $E(K^T\underline{b}^0 - \underline{m}) =$

$K^T\underline{b} - \underline{m}$. $Var(K^T\underline{b}^0 - \underline{m}) = Var(K^T\underline{b}^0) = \sigma^2 K^T G K \Rightarrow \frac{1}{\sigma}(K^T\underline{b}^0 - \underline{m}) \sim N\left[\frac{1}{\sigma}(K^T\underline{b} - \underline{m}, K^T G K\right] \Rightarrow \frac{Q}{\sigma^2} \sim \chi^{2'}\left[r(K), \frac{1}{2\sigma^2}(K^T\underline{b} - \underline{m})^T (K^T G K)^{-1}(K^T\underline{b} - \underline{m})\right]$. Also, $\frac{1}{\sigma}(I - P_x)\underline{y} \sim N(\underline{0}, I - P_x) \Rightarrow SS(E) \sim \chi^2(r(I - P_x), 0) \sim \chi^2(N - r(X))$. Showing Q and $SS(E)$ are independent is similar to that in Chapter 3.

Theorem 5.2: For the linear model $\underline{y} = X\underline{b} + \underline{e}$ where $\underline{e} \sim N(\underline{0}, \sigma^2 I)$, the likelihood ratio test statistic for testing $H : K^T\underline{b} = \underline{m}$ is

$$L = \frac{(K^T\underline{b} - \underline{m})^T (K^T G K)^{-1}(K^T\underline{b} - \underline{m})}{\underline{y}^T (I - P_x)\underline{y}} \times \frac{N - r(X)}{r(K)}$$

and $L \sim F'\left[r(K), N - r(X), \frac{1}{2\sigma^2}(K^T\underline{b} - \underline{m})^T (K^T G K)^{-1}(K^T\underline{b} - \underline{m})\right]$ where K^T has full row rank and $\Re(K^T) \subseteq \Re(X)$. The test statistic for H_0 is

$$F = \frac{(K^T\underline{b}^0 - \underline{m})^T (K^T (X^T X)^- K)^{-1}(K^T\underline{b}^0 - \underline{m})}{\underline{y}^T (I - P_x)\underline{y}} \times \frac{N - r(X)}{r(K)}$$

This can be found in 5.5a,b of the text book. The test for regression in the full rank case $H : \underline{b} = \underline{0}$ will test $H : X\underline{b} = \underline{0}$ (pick out a full rank set of rows in X). But, X is not of full column rank, so we must restate the hypothesis in order to use Theorem 5.2. Suppose that $r_1, r_2, ..., r_{r(X)}$ are the indices of a set of LIN rows of matrix X. Define $R^T_{r(X)\times N}$ by

$$\left(R^T\right)_{ij} = \begin{cases} 1 & \text{if } j = r_i,\ i = 1, ..., r(X),\ j = 1, 2, ..., N. \\ 0 & \text{otherwise.} \end{cases}$$

The $i - th$ row of R^T picks out the $r_i - th$ row of X. Then $X\underline{b} = \underline{0}$ iff $R^T X\underline{b} = \underline{0}$. So, our hypothesis can be stated as $H : K^T\underline{b} = \underline{0}$ where $K^T = R^T X$, and K^T has full rank $s = r(X)$. Therefore, $Q = (K^T\underline{b}^0 - \underline{m})^T (K^T(X^T X)^- K)^{-1}(K^T\underline{b}^0 - \underline{m}) = (R^T X\underline{b}^0)(R^T X(X^T X)^- X^T R)^{-1}(R^T X\underline{b}^0) = \underline{y}^T X(X^T X)^- X^T R(R^T X(X^T X)^- X^T R)^{-1}\ (R^T X\ (X^T X)^- X^T\underline{y}) = \underline{y}^T\ \overbrace{P_x R(R^T P_x R)^{-1} R^T P_x}^{=A_H}\ \underline{y}$, $P_x = X(X^T X)^- X^T$. Proof: Show that $P_x = A_H$. We know P_x is idempotent and A_H is idempotent. Consider $P_x A_H$. Then, $P_x A_H = A_H = A_H^2$. Hence, $(P_x - A_H)(P_x - A_H) = P_x^2 - A_H P_x - P_x A_H + A_H^2 = P_x - A_H - A_H + A_H = P_x - A_H \Rightarrow P_x - A_H$ is idempotent. Also, $r(P_x) = r(X)$ and $r(A_H) = r(K) = r(X) \Rightarrow r(P_x - A_H) = tr(P_x - A_H) = tr(P_x) - tr(A_H) = r(P_x) - r(A_H) = r(X) - r(X) = 0 \Rightarrow P_x - A_H = 0$ i.e. $P_x = A_H$. So, we see that $SS(R) = \underline{y}^T P_x\underline{y}$ is the Q for testing the overall regression hypothesis $H : X\underline{b} = \underline{0}$. If X contains a column of 1's (the model contains a general mean term) then we may, as in the regression case, isolate a component of $SS(R)$ for testing the mean $SS(R) = \underline{y}^T P_x\underline{y} = \underline{y}^T(P_x - \frac{1}{N}J)\underline{y} + \underline{y}^T(\frac{1}{N}J)\underline{y} = SS(R)_m + SS(m)$. These two quadratic forms are independent since $(P_x - \frac{1}{N}J)\sigma^2 I(\frac{1}{N}J) = \sigma^2(\frac{1}{N}P_x J) - \sigma^2\frac{1}{N^2}JJ = \sigma^2\frac{1}{N}J - \sigma^2\frac{1}{N}J = 0$. Note that this fails if X does not contain a column of 1's. Hence our ANOVA table is

SS	d.f.
$SS(m) = \underline{y}^T\frac{1}{N}J\underline{y}$	1
$SS(R)_m = \underline{y}^T(P_x - \frac{1}{N}J)\underline{y}$	$r(X) - 1$
$SS(E) = \underline{y}^T(I - P_x)\underline{y}$	$N - r(X)$
$SS(Total) = \underline{y}^T\underline{y}$	N

or some variant thereof. See tables 5.5, 5.6a, 5.6b on pages 176 and 177 of the text book. What do these test? By looking at the non-centralities, we can show that $SS(m)$ is Q for testing $H : E(\bar{y}) = \underline{0}$ where $\bar{y} = \frac{1}{N}\sum_{i=1}^N y_i$ i.e. $H : \underline{j}^T X\underline{b} = 0$. $SS(R)_m$ is Q for testing $H : \mu_1 = \mu_2 = \cdots = \mu_N$ where $\mu_i = E(y_i)$.

15.17.1 A Reduced Model

This section covers the reduced model corresponding to $H : K^T\underline{b} = \underline{m}$ (Section 5.5c of the text book). In our discussion of the likelihood ratio test statistic for $H : K^T\underline{b} = \underline{m}$, we have seen a solution to the normal equations for the reduced model corresponding to H is $\underline{b}_H^0 = \underline{b}^0 - GK(K^TGK)^{-1}(K^T\underline{b}^0 - \underline{m})$ where $\underline{b}^0 = GX^T\underline{y}$ is a solution in the full model and G is a g-inverse of X^TX. We went on to derive the sums of squares for testing H as $Q = (\underline{y} - X\underline{b}_H^0)^T(\underline{y} - X\underline{b}_H^0) - (\underline{y} - X\underline{b}^0)^T(\underline{y} - X\underline{b}^0) = SS(E)_{red} - SS(E)_{full}$ showing that Q is the *reduction in error* from the reduced model to the full model. As in Chapter 3, we now look to see if we can make a similar statement about $SS(R)$. $Q = (K^T\underline{b}^0 - \underline{m})^T(K^TGK)^{-1}(K^T\underline{b}^0 - \underline{m}) = (K^TGX^T\underline{y} - \underline{m})^T(K^TGK)^{-1}(K^TGX^T\underline{y} - \underline{m}) = (\underline{y} - \underline{m}_1)^T\overbrace{XG^TK(K^TGK)^{-1}K^TGX^T}^{=A_H}(\underline{y} - \underline{m}_1) = (\underline{y} - \underline{m}_1)^TA_H(\underline{y} - \underline{m}_1)$ where $\underline{m}_1 = XK(K^TK)^{-1}\underline{m}$. Now $\underline{m}_1 = \underline{0}$ iff $\underline{m} = \underline{0}$ (need to prove) and when this is true, $Q = \underline{y}^TA_H\underline{y}$. We already have $Q = SS(E)_{red} - SS(E)_{full}$ which for $H : K^T\underline{b} = \underline{0}$ is $\underline{y}^TA_H\underline{y} = SS(E)_{red} - \underline{y}^T(I - P_x)\underline{y}$ or $\underline{y}^T\underline{y} - SS(E))_{red} = \underline{y}^T(P_x - A_H)\underline{y}$ i.e. $SS(Total)_{red} - SS(E)_{red} = \underline{y}^T(P_x - A_H)\underline{y} \Rightarrow SS(R)_{reduced} = \underline{y}^T(P_x - A_H)\underline{y}$. Hence, for $H : K^T\underline{b} = \underline{0}$, $SS(R)_{full} = \underline{y}^TP_x\underline{y} = \underline{y}^T(P_x - A_H)\underline{y} + \underline{y}^TA_H\underline{y} = SS(R)_{red} + Q \Rightarrow Q = SS(R)_{full} - SS(R)_{red} \Rightarrow Q$ is the gain in regression sum of squares from the reduced model to the full model. Just as in Chapter 3 of the text book for the full rank case, this argument fails if $\underline{m} \neq \underline{0}$, since then the reduced model has a different $SS(T)$.

15.17.2 Non-Estimable Functions

This section covers Section 5.5(d) in the text book. Question: what happens when we try to test $K^T\underline{b} = \underline{m}$ when the functions $K^T\underline{b}$ are not estimable? Proceeding as before, we minimize $(\underline{y} - X\underline{b})^T(\underline{y} - X\underline{b})$ subject to $K^T\underline{b} = \underline{m}$ where the rows of K^T are LIN of the rows of X (not in row space of X). $F = \underline{y}^T\underline{y} - 2\underline{b}^TX^T\underline{y} + \underline{b}^TX^TX\underline{b} + 2(\underline{b}^TK - \underline{m}^T)\underline{\theta}$. $\frac{1}{2}\frac{dF}{d\underline{b}} = -X^T\underline{y} + X^TX\underline{b} + K\underline{\theta} = \underline{0} \Rightarrow X^TX\underline{b}_H^0 = X^T\underline{y} - K\underline{\theta}$ and $K^T\underline{b}_H^0 = \underline{m}$. We will show there is a solution at $\underline{\theta} = \underline{0}$. Hence, we must find $\underline{b}_H^0$ such that $X^TX\underline{b}_H^0 = X^T\underline{y}$ and $K^T\underline{b}_H^0 = \underline{m}$. Consider the equations $K^T(\overbrace{GX^TX}^{=H} - I)\underline{z} = \underline{m} - K^TGX^T\underline{y}$ where G is the g-inverse of X^TX. Let $\underline{z}_1$ be any solution, and take $\underline{b}_H^0 = GX^T\underline{y} + (H - I)\underline{z}_1$. Then, $K^T\underline{b}_H^0 = K^TGX^T\underline{y} + K^T(H - I)\underline{z}_1 = K^TGX^T\underline{y} + \underline{m} - K^TGX^T\underline{y} = \underline{m}$ and $X^TX\underline{b}_H^0 = X^T\overbrace{XGX^T}^{=P_x}\underline{y} + \overbrace{X^TX[(X^TX)^-(X^TX) - I]}^{=0}\underline{z}_1 = X^T\underline{y}$ because $X^TP_x = X^T$. Therefore, $\min_{K^T\underline{b} = \underline{m}}(\underline{y} - X\underline{b})^T(\underline{y} - X\underline{b}) = SS(E)$ for the full model since our $\underline{b}_H^0$ satisfies the usual equations. Therefore, $Q = SS(E)_{red} - SS(E)_{full} = SS(E)_{full} - SS(E)_{full} = 0$. Therefore, our method for deriving the test statistic fails. We cannot test $K^T\underline{b} = \underline{m}$ when $K^T\underline{b}$ is not estimable. Other consequences include:

1. We can check the *testability* of $K^T\underline{b} = \underline{m}$ by checking the estimability of $K^T\underline{b}$. So, check $K^TH = K^T$.
2. Imposing non-estimable constraints when solving the normal equations still gives a valid solution. We can do this whenever it makes the problem easier.

15.17.3 Orthogonal Contrasts and Decomposition of $SS(R)$

This section covers Section 5.5(g) of the text book. Let $H : K^T\underline{b} = \underline{0}$ be a testable hypothesis of orders. The sums of squares for testing H is $Q = (K^T\underline{b}^0)^T(K^TGK)^{-1}(K^T\underline{b}^0)$. Let's write

$$K^T = \begin{pmatrix} \underline{k}_1^T \\ \underline{k}_2^T \\ \vdots \\ \underline{k}_s^T \end{pmatrix}$$

to display its rows. Then, $K^T\underline{b} = \underline{0}$ is $H_1 : \underline{k}_1^T\underline{b} = 0$, $H_2 : \underline{k}_2^T\underline{b} = 0, \ldots,$ $H_s : \underline{k}_s^T\underline{b} = 0$. Write $q_i = (\underline{k}_i^T\underline{b}^0)^T(\underline{k}_i^TG\underline{k}_i)^{-1}(\underline{k}_i^T\underline{b}^0)$. Then, q_i is the sums of squares for testing $H_i : \underline{k}_i^T\underline{b} = 0$. Since H is simultaneously testing H_i for $i = 1, 2, ..., s$ could it be that $Q = \sum_{i=1}^{s} q_i$? This is true if certain conditions hold on $\underline{k}_i$. In fact if $\underline{k}_i^T G\underline{k}_j = 0, \forall i \neq j \Rightarrow Q = \sum_{i=1}^{s} q_i$. This is easily seen as follow. $\underline{k}_i^T G\underline{k}_j$ is the (i,j)-th element of $K^T GK$. $\underline{k}_i^T G\underline{k}_j = 0, \forall i \neq j \Rightarrow K^T GK = Diag(\underline{k}_i^T G\underline{k}_i) \Rightarrow (K^T GK)^{-1} = Diag((\underline{k}_i^T G\underline{k}_i)^{-1}) \Rightarrow$

$$Q = (K^T \underline{b}^0)^T (K^T GK)^{-1} (K^T \underline{b}^0) = (\underline{k}_1^T \underline{b}^0, \underline{k}_2^T \underline{b}^0, ..., \underline{k}_s^T \underline{b}^0) Diag((\underline{k}_i^T G\underline{k}_i)^{-1}) \begin{pmatrix} \underline{k}_1^T \underline{b}^0 \\ \underline{k}_2^T \underline{b}^0 \\ \vdots \\ \underline{k}_s^T \underline{b}^0 \end{pmatrix} =$$

$\sum_{i=1}^{s} (\underline{k}_i \underline{b}^0)(\underline{k}_i^T G\underline{k}_i)^{-1}(\underline{k}_i^T \underline{b}^0) = \sum_{i=1}^{s} q_i$. In fact, the $\underline{q}_i's$ are independent iff $\underline{k}_i^T G\underline{k}_j = 0, \forall i \neq j$ by Theorem 2.7. If $\underline{k}_i^T \underline{b}$ for $i = 1, 2, ..., s$ are such that $\underline{k}_i^T G\underline{k}_j = 0, \forall i \neq j$, then they are called *orthogonal linear functions* of $\underline{b}$. Searle also calls them *orthogonal contrasts,* though most authors save the term "contrasts" for $\underline{k}_i's$ which also satisfy $\underline{k}_i^T \underline{j} = 0$. Suppose $s = r(X)$. Then, $Q = SS(R)$ and we say the $q_i's$ *decompose* $SS(R)$ into sums of squares with 1 degrees of freedom each. $SS(R) = \sum_{i=1}^{r(X)} q_i$. Likewise, if $s = r(X) - 1$, then a set of $q_i's$ adding to $SS(R)_m$ is to decompose $SS(R)_m$.

15.17.4 Using Constraints to Find Solutions

This section covers Section 5.7(a) in the text book. Let C be such that $C^T \underline{b}$ are LIN, non-estimable functions. We now note that if we minimize $(\underline{y} - X\underline{b})^T (\underline{y} - X\underline{b})$ subject to $C^T \underline{b} = \underline{\delta}$, the solution will be to the normal equations. Doing this with Lagrange multipliers, we obtain $X^T X\underline{b} + C\underline{\theta} = X^T \underline{y}$ and $C^T \underline{b} = \underline{\delta}$ i.e.

$$\begin{pmatrix} X^T X & C \\ C^T & 0 \end{pmatrix} \begin{pmatrix} \underline{b} \\ \underline{\theta} \end{pmatrix} = \begin{pmatrix} X^T \underline{y} \\ \underline{\delta} \end{pmatrix}$$

If we choose C^T to have $p - r$ rows where X is $n \times p$ of rank r, then the left-hand matrix is $(2p - r) \times (2p - r)$ of rank $2p - r = (p - r) + (p - r) + (r)$. So we can invert a non-singular matrix to find a solution $\underline{b}^0$. This *does not* mean that we think $C^T \underline{b} = \underline{\delta}$. That is, we are not placing restrictions on the parameters. We are simply using a technique for finding a solution which happens to satisfy $C^T \underline{b}^0 = \underline{\delta}$. This is discussed on pages 209 and 212 of the text book.

15.18 Homework and Answers

In the textbook on pages 132-134, work problems 6, 9, and 19. In problem 19, use the intercept model only. The author's matrix P is our $I - P_X$. That is, $P = I - P_X = I - X(X'X)^{-1}X'$.

6. $SS(m)$, SSR_m, $SS(E)$.

$$SS(E) = \underline{y}^T (I - P_x)\underline{y}. \qquad \frac{1}{\sigma^2} SS(E) = \chi^2 \left[n - (k+1), \frac{(X\underline{b})^T (I - P_x) X\underline{b}}{2\sigma^2} \right]$$

$A = \frac{1}{\sigma^2}(I - P_x)$. $V = \sigma^2 I$. $AV = I - P_x$ is idempotent. $E(\underline{y}) = X\underline{b} \sim \chi^2(n - (k+1), 0)$. $SS(T) = \underline{y}^T \underline{y}$. $A = \frac{1}{\sigma^2} I$. $V = \sigma^2 I$. $\frac{1}{\sigma^2} SS(T) \sim \chi^2 \left[n, \frac{1}{2\sigma^2}(X\underline{b})^T (X\underline{b}) \right]$. $SS(R) = \underline{y}^T P_x \underline{y}$. $\frac{1}{\sigma^2} SS(R) \sim \chi^2 \left[k+1, \frac{1}{2\sigma^2}(X\underline{b})^T P_x (X\underline{b}) \right]$. So, non-centrality of $SS(R)$ plus non-centrality of $SS(E)$ is equal to the non-centrality of $SS(T)$. So, $\frac{1}{2\sigma^2}(X\underline{b})^T (X\underline{b}) + 0 = \frac{1}{2\sigma^2}(X\underline{b})^T (X\underline{b}) = \frac{1}{\sigma^2} SS(T)$. Show that the non-centrality of $SS(m)$ plus the non-centrality of $SS(R)_m$ equals to the non-centrality of $SS(R)$. $SS(R)_m = \underline{y}^T A_H \underline{y}$ where A_H is the A matrix of the quadratic form Q for testing $H : b_1 = b_2 = \cdots = b_k = 0$. $SS(m) = \underline{y}^T (P_x - A_H)\underline{y}$. Hence, $\frac{1}{\sigma^2} SS(R)_m = \frac{1}{2\sigma^2}(X\underline{b})^T A_H (X\underline{b})$. Hence, $\frac{1}{\sigma^2} SS(m) = \frac{1}{2\sigma^2}(X\underline{b})^T (P_x - A_H)(X\underline{b})$.

9. The hypothesis has rank 2.

$$K^T = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix}, \ \underline{m} = \begin{pmatrix} 4 \\ 3 \end{pmatrix}.$$

$K^T\underline{b} = \underline{m}$ says $b_1 - b_2 = 4$ and $b_2 - b_3 = 3$ i.e. $b_1 = b_2 + 4$ and $b_2 = b_3 + 3$. So, $b_2 + 4 = b_3 + 7$.

19. $Cov(\underline{\widehat{e}}, \underline{y}) = Cov((I - P_X)\underline{y}, \underline{y})$. Since $\widehat{e} = \underline{y} - \widehat{\underline{y}} = (I - P_X)\underline{y} = (I - P_X)Cov(\underline{y}, \underline{y})$ since $Cov(A\underline{y}, B\underline{y}) = ACov(\underline{y}, \underline{y})B^T$. Then we have, $(I - P_X)Var(\underline{y}) = (I - P_X)\sigma^2 I = \sigma^2(I - P_x)$. $Cov(\underline{\widehat{e}}, \underline{\widehat{b}}) = Cov((I - P_X)\underline{y}, (X^TX)^{-1}X^T\underline{y}) = (I - P_X)Cov(\underline{y}, \underline{y})X(X^TX)^{-1} = \sigma^2 \overbrace{(I - P_X)X}^{=0}(X^TX)^{-1} = 0$. $Cov(\underline{e}, \underline{\widehat{b}}) = Cov(\underline{y} - X\underline{b}, (X^TX)^{-1}X^T\underline{y}) = Cov(\underline{y}, (X^TX)^{-1}X^T\underline{y}) = Cov(\underline{y}, \underline{y})X(X^TX)^{-1} = \sigma^2X(X^TX)^{-1}$.

Problems 1-6 below refer to this model and data. Here are eight measurements on the variables y, x_1, x_2, and x_3. The model is $y = b_0 + b_1x_1 + b_2x_2 + b_3x_3 + \epsilon$ with $\epsilon \sim N(\underline{0}, \sigma^2 I)$.

$$\begin{pmatrix} y & x_1 & x_2 & x_3 \\ 3 & 0 & -1 & -2 \\ 11 & 0 & 2 & 0 \\ 4 & 1 & -3 & -1 \\ 16 & 1 & 2 & 3 \\ 7 & 2 & -1 & 1 \\ 16 & 2 & 0 & 2 \\ 17 & 3 & -1 & 4 \\ 1 & 3 & 2 & -3 \end{pmatrix}$$

1. Find $\widehat{\underline{b}}$, $SS(E)$, $SS(R)$, $SS(M)$, $SSR(M)$, and $SS(T)$. $SS(R) = yP_x\underline{y} = \underline{y}^TX(X^TX)^{-1}X^T\underline{y} = \widehat{\underline{b}}^T X^T\underline{y}$. $SS(E) = \underline{y}^T(I - P_x)\underline{y} = \underline{y}^T\underline{y} - SS(R) = SS(T) - SS(R)$. $SS(m) = \frac{1}{n}\left(\sum_{i=1}^n y_i\right)^2$.

$$P_X = \begin{pmatrix} 0.4693 & 0.2556 & 0.3805 & -0.00524 & 0.081 & -0.00537 & -0.155 & 0.0049 \\ 0.2556 & 0.5184 & -0.0581 & 0.3842 & -0.0318 & 0.05793 & -0.1407 & 0.03991 \\ 0.3805 & -0.05813 & 0.5648 & -0.1873 & 0.2172 & 0.0604 & 0.1133 & -0.0657 \\ -0.0053 & 0.3842 & -0.1873 & 0.5083 & 0.034 & 0.187 & 0.1833 & -0.0792 \\ 0.0806 & -0.0319 & 0.21713 & 0.03396 & 0.1932 & 0.1579 & 0.2843 & 0.0896 \\ -0.00544 & 0.0579 & 0.0604 & 0.187 & 0.1579 & 0.1895 & 0.3122 & 0.0654 \\ -0.1802 & -0.1661 & 0.08797 & 0.158 & 0.259 & 0.2287 & 0.6083 & -0.0043 \\ 0.00483 & 0.03981 & -0.0658 & -0.0792 & 0.0896 & 0.0654 & -0.0043 & 0.9741 \end{pmatrix}$$

$$X^TX = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 2 & 2 & 3 & 3 \\ -1 & 2 & -3 & 2 & -1 & 0 & -1 & 2 \\ -2 & 0 & -1 & 3 & 1 & 2 & 4 & -3 \end{pmatrix} \begin{pmatrix} 1 & 0 & -1 & -2 \\ 1 & 0 & 2 & 0 \\ 1 & 1 & -3 & -1 \\ 1 & 1 & 2 & 3 \\ 1 & 2 & -1 & 1 \\ 1 & 2 & 0 & 2 \\ 1 & 3 & -1 & 4 \\ 1 & 3 & 2 & -3 \end{pmatrix} = \begin{pmatrix} 8 & 12 & 0 & 4 \\ 12 & 28 & 0 & 11 \\ 0 & 0 & 24 & 0 \\ 4 & 11 & 0 & 44 \end{pmatrix}.$$

$$(X^TX)^{-1} = \begin{pmatrix} 0.3516 & -0.153165 & 0 & 0.00633 \\ -0.1532 & 0.10633 & 0 & -0.01266 \\ 0 & 0 & 0.0417 & 0 \\ 0.00633 & -0.01266 & 0 & 0.02532 \end{pmatrix}.$$

$$\underline{\widehat{b}} = (X^T X)^{-1} X^T \underline{y} = \begin{pmatrix} 8.888 \\ -0.5288 \\ 0.7089 \\ 2.55099 \end{pmatrix}.$$

$SS(E) = \underline{y}^T [I - P_X] \underline{y} = \underline{y}^T I \underline{y} - \underline{y}^T P_X \underline{y} = (\underline{y} - \underline{\widehat{y}})^T (\underline{y} - \underline{\widehat{y}}) = \sum_{i=1}^{8} (y_i - \widehat{y}_i)^2 = 19.232$. $SS(R) = SS(T) - SS(E) = 997 - 19.232 = 977.768$. $SS(T) = \underline{y}^T \underline{y} = \sum_{i=1}^{8} y_i^2 = 997$. $SS(mean) = N\bar{y}^2 = 703.125$. $SSR(M) = SS(R) - SS(M) = 997.768 - 703.125 = 274.64$.

2. Test $b_1 = b_2 = b_3 = 0$.

$$K = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad r(K) = 3.$$

$r(X) = 4$. The test statistic is

$$\frac{SSR(M)/df1}{SS(E)/df2} \sim F(df1, df2), \quad \frac{274.64/3}{19.232/4} = 19.04 = F_{obs}, \quad F_{0.05}(3,4) = 6.59 \Rightarrow \text{ reject } H_0.$$

We can conclude that at least one b_i does not equal to zero.

3. This problem requires calculating the quadratic forms Q that appear in the numerator of the test statistics for testing several different linear hypotheses. $H : \underline{b}_q = \underline{0}$. T_{qq} is the sub-matrix of $(X^T X)^{-1}$ corresponding to the elements of $\underline{b}_q$. $Q = \widehat{\underline{b}}_q^T (T_{qq})^{-1} \widehat{\underline{b}}_q$. This answer has precision issues to the right of the decimal place.

   (a) Consider the null hypotheses $H_1 : b_1 = b_3 = 0$ and $H_2 : b_2 = 0$. Calculate Q_1 and Q_2 where Q_i is the quadratic form Q for testing H_i. Show that $Q_1 + Q_2 = SSR(M)$.

$$K^T = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \underline{m} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

$$K^T \underline{\widehat{b}} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 8.888 \\ -0.5288 \\ 0.7089 \\ 2.55099 \end{pmatrix} = \begin{pmatrix} -0.5288 \\ 2.55099 \end{pmatrix}.$$

$$(K^T \underline{\widehat{b}} - \underline{m}) = \begin{pmatrix} -0.5288 \\ 2.55099 \end{pmatrix}.$$

$$K^T (X^T X)^{-1} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0.3516 & -0.153165 & 0 & 0.00633 \\ -0.1532 & 0.10633 & 0 & -0.01266 \\ 0 & 0 & 0.0417 & 0 \\ 0.00633 & -0.01266 & 0 & 0.02532 \end{pmatrix} =$$

$$\begin{pmatrix} -0.1532 & 0.10633 & 0 & -0.01266 \\ 0.00633 & -0.01266 & 0 & 0.02532 \end{pmatrix}.$$

$$K^T(X^TX)^{-1}K = \begin{pmatrix} -0.1532 & 0.10633 & 0 & -0.01266 \\ 0.00633 & -0.01266 & 0 & 0.02532 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{pmatrix} =$$

$$\begin{pmatrix} 0.10633 & -0.01266 \\ -0.01266 & 0.02532 \end{pmatrix}.$$

Now to find the inverse of $K^T(X^TX)^{-1}K$.

$$\left(\begin{array}{cc|cc} 0.10633 & -0.01266 & 1 & 0 \\ -0.01266 & 0.02532 & 0 & 1 \end{array}\right)$$

$$\left(\begin{array}{cc|cc} 1 & -0.1191 & 9.405 & 0 \\ -0.01266 & 0.02532 & 0 & 1 \end{array}\right) \to 0.01266R_1 + R_2 = R_2$$

$$\left(\begin{array}{cc|cc} 1 & -0.1191 & 9.405 & 0 \\ 0 & 0.02381 & 0.1191 & 1 \end{array}\right) \to$$

$$\left(\begin{array}{cc|cc} 1 & -0.1191 & 9.405 & 0 \\ 0 & 1 & 5 & 42 \end{array}\right) \to 0.1191R_2 + R_1 = R_1$$

$$\left(\begin{array}{cc|cc} 1 & 0 & 10 & 5 \\ 0 & 1 & 5 & 42 \end{array}\right) \Rightarrow (K^T(X^TX)^{-1}K)^{-1} = \begin{pmatrix} 10 & 5 \\ 5 & 42 \end{pmatrix}.$$

Finally find $(K^T\widehat{\underline{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1}$.

$$(K^T\widehat{\underline{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1} = (-0.5288,\ 2.55099) \begin{pmatrix} 10 & 5 \\ 5 & 42 \end{pmatrix} = (7.467,\ 104.5).$$

Now find $(K^T\widehat{\underline{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1}(K^T\widehat{\underline{b}} - \underline{m})$.

$$(K^T\widehat{\underline{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1}(K^T\widehat{\underline{b}} - \underline{m}) = (7.467,\ 104.5) \begin{pmatrix} -0.5288 \\ 2.55099 \end{pmatrix} = 262.60 = Q_1.$$

Now, do similar calculations for the hypothesis $H_2 : b_2 = 0$.

$$K = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad \underline{m} = 0.$$

$$K^T\widehat{\underline{b}} = (0, 0, 1, 0) \begin{pmatrix} 8.888 \\ -0.5288 \\ 0.7089 \\ 2.55099 \end{pmatrix} = 0.7089.$$

$K^T\underline{\widehat{b}} - \underline{m} = 0.7089$.

$$K^T(X^TX)^{-1} = (0,\ 0,\ 1,\ 0)\begin{pmatrix} 0.3516 & -0.153165 & 0 & 0.00633 \\ -0.1532 & 0.10633 & 0 & -0.01266 \\ 0 & 0 & 0.0417 & 0 \\ 0.00633 & -0.01266 & 0 & 0.02532 \end{pmatrix} = (0,\ 0,\ 0.0417,\ 0).$$

Find $K^T(X^TX)^{-1}K$.

$$K^T(X^TX)^{-1}K = (0,\ 0,\ 0.0417,\ 0).\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = 0.0417 \Rightarrow (K^T(X^TX)^{-1}K)^{-1} = 24.$$

Find $(K^T\underline{\widehat{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1}$. $(K^T\underline{\widehat{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1} = (0.7089)(24) = 17$. Find $(K^T\underline{\widehat{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1}(K^T\underline{\widehat{b}} - \underline{m})$. $(K^T\underline{\widehat{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1}(K^T\underline{\widehat{b}} - \underline{m}) = (17)(0.7089) = 12.0417 = Q_2$. $Q_1 + Q_2 = 262.60 + 12.0417 = 274.6417$.

(b) Consider the null hypotheses $H_3 : b_2 = b_3 = 0$ and $H_4 : b_1 = 0$. Calculate Q_3 and Q_4, and show that $Q_3 + Q_4 \neq SSR(M)$.

$$K^T = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},\ \underline{m} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

$$K^T\underline{\widehat{b}} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 8.888 \\ -0.5288 \\ 0.7089 \\ 2.55099 \end{pmatrix} = (0.7089,\ 2.55099).$$

$(K^T\underline{\widehat{b}} - \underline{m})^T = (0.7089,\ 2.55099)$.

$$K^T(X^TX)^{-1} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 0.3516 & -0.153165 & 0 & 0.00633 \\ -0.1532 & 0.10633 & 0 & -0.01266 \\ 0 & 0 & 0.0417 & 0 \\ 0.00633 & -0.01266 & 0 & 0.02532 \end{pmatrix} =$$

$$\begin{pmatrix} 0 & 0 & 0.0417 & 0 \\ 0.00633 & -0.01266 & 0 & 0.02532 \end{pmatrix}.$$

$$K^T(X^TX)^{-1}K = \begin{pmatrix} 0 & 0 & 0.0417 & 0 \\ 0.00633 & -0.01266 & 0 & 0.02532 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0.0417 & 0 \\ 0 & 0.02532 \end{pmatrix}.$$

$$(K^T(X^TX)^{-1}K)^{-1} = \begin{pmatrix} 24 & 0 \\ 0 & 39.5 \end{pmatrix}.$$

$$(K^T\underline{\widehat{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1} = (0.7089,\ 2.55099)\begin{pmatrix} 24 & 0 \\ 0 & 39.5 \end{pmatrix} = (17,\ 100.76).$$

$$(K^T\underline{\widehat{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1}(K^T\underline{\widehat{b}} - \underline{m}) = (17,\ \ 100.76)\begin{pmatrix} 0.7089 \\ 2.55099 \end{pmatrix} = 269.02 = Q_3.$$

Now under $H_4 : b_1 = 0$,

$$K^T = (0,\ \ 1,\ \ 0,\ \ 0),\ \ \underline{m} = 0.$$

$$K^T\underline{\widehat{b}} = (0,\ \ 1,\ \ 0,\ \ 0)\begin{pmatrix} 8.888 \\ -0.5288 \\ 0.7089 \\ 2.55099 \end{pmatrix} = -0.5288.$$

$K^T\underline{\widehat{b}} - \underline{m} = -0.5288.$

$$K^T(X^TX)^{-1} = (0,\ \ 1,\ \ 0,\ \ 0)\begin{pmatrix} 0.3516 & -0.153165 & 0 & 0.00633 \\ -0.1532 & 0.10633 & 0 & -0.01266 \\ 0 & 0 & 0.0417 & 0 \\ 0.00633 & -0.01266 & 0 & 0.02532 \end{pmatrix} =$$

$$(-0.1532,\ \ 0.10633,\ \ 0,\ \ -0.01266).$$

$$K^T(X^TX)^{-1}K = (-0.1532,\ \ 0.10633,\ \ 0,\ \ -0.01266)\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = 0.10633 \Rightarrow (K^T(X^TX)^{-1}K)^{-1} = 9.405.$$

$(K^T\underline{\widehat{b}} - \underline{m})^T(K^T(X^TX)^{-1}K)^{-1}(K^T\underline{\widehat{b}} - \underline{m}) = (-0.5288)(9.405)(-0.5288) = 2.595 = Q_4$. $Q_3 + Q_4 = 269.02 + 2.595 = 271.65 \neq SSR(M)$.

(c) Why do the two quadratic forms add up in 3(a) but not in 3(b)? Generalize. Q_1 and Q_2 are independent chi-squares. Q_3 and Q_4 are not independent chi-squares. $Q_i = \underline{y}^T A_{H_i}\underline{y}$. Q_1 and Q_2 are independent iff $A_{H_1}(\sigma_2 I)A_{H_2} = 0$ i.e. iff $A_{H_1}A_{H_2} = 0$. $A_{H_i} = X\ (X^TX)^{-1}K_i(K_i^T\ (X^TX)^{-1}K_i^T$ $(X^TX)^{-1}X^T$. Then, $A_{H_1}A_{H_2} = X(X^TX)^{-1}K_1(K_1\ (X^TX)^{-1}\ K_1)^{-1}\ \overbrace{K_1^T(X^TX)^{-1}K_2}^{=0}\ (K_2^T\ (X^TX)^{-1}K_2)^{-1}\ K_2^T(X^T\ X)^{-1}X^T$. If

$$(X^TX)^{-1} = \begin{pmatrix} w_1 & 0 \\ 0 & w_2 \end{pmatrix}\begin{matrix} \} & q \text{ of these} \\ \} & k+1-q \text{ of these} \end{matrix}$$

$\underline{b}_q$ is the first q elements and $\underline{b}_p$ is the other $k+1-q$ elements. If $K_1^T\underline{b} = \underline{b}_q$ and $K_2^T\underline{b} = \underline{b}_p$, then $K_1^T(X^TX)^{-1}K_2 = 0$.

4. Consider the reduced model given by the restriction $b_1 = 0$. Calculate $SSR(reduced)$ and $SSE(reduced)$ by

(a) Deleting the appropriate column from X and calculating $SS(R)$ and $SS(E)$ from the new X in the usual way.

$$X^TX = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & 2 & -3 & 2 & -1 & 0 & -1 & 2 \\ -2 & 0 & -1 & 3 & 1 & 2 & 4 & -3 \end{pmatrix} \begin{pmatrix} 1 & -1 & -2 \\ 1 & 2 & 0 \\ 1 & -3 & -1 \\ 1 & 2 & 3 \\ 1 & -1 & 1 \\ 1 & 0 & 2 \\ 1 & -1 & 4 \\ 1 & 2 & -3 \end{pmatrix} = \begin{pmatrix} 8 & 0 & 4 \\ 0 & 24 & 0 \\ 4 & 0 & 44 \end{pmatrix} \Rightarrow$$

$$(X^TX)^{-1} = \begin{pmatrix} 0.13095 & 0 & -0.01191 \\ 0 & 0.0417 & 0 \\ -0.0119 & 0 & 0.02381 \end{pmatrix}.$$

$$(X^TX)^{-1}X^T = \begin{pmatrix} 0.15475 & 0.13095 & 0.1429 & 0.09522 & 0.11904 & 0.10713 & 0.08331 & 0.1667 \\ -0.0417 & 0.0834 & -0.1251 & 0.0834 & -0.0417 & 0 & -0.0417 & 0.0834 \\ -0.05952 & -0.0119 & -0.03571 & 0.05953 & 0.01191 & 0.03572 & 0.08334 & 0.08333 \end{pmatrix}$$

$$(X^TX)^{-1}X^T\underline{y} = \begin{pmatrix} 8.13015 \\ 0 \\ 0.7089 \\ 2.488 \end{pmatrix} = \widehat{\underline{b}}.$$

Finally calculate, $\widehat{\underline{y}} = X\widehat{\underline{b}}$.

(b) Using Q_4 from Problem 3 and the sums of squares from Problem 1. $Q_4 = 2.595$. If $Q_4 = SS(E)_{reduced} - SS(E)_{full}$, then $2.595 = SS(E)_{reduced} - 19.232 \Rightarrow SS(E)_{reduced} = 21.827$. $SS(T)_{full} = SS(E)_{reduced} + SS(R)_{reduced} \Rightarrow 997 = 21.827 + SS(R)_{reduced} \Rightarrow SS(R)_{reduced} = 975.173$.

(c) Using $\widetilde{\underline{b}} = \widehat{\underline{b}} - (X'X)^{-1}K(K'(X'X)^{-1}K)^{-1}(K'\widehat{\underline{b}} - \underline{m})$.

$$(X^TX)^{-1}K(K^T(X^TX)^{-1}K)^{-1}(K^T\widehat{\underline{b}} - \underline{m}) = \begin{pmatrix} 0.7617 \\ -0.5288 \\ 0 \\ -0.063 \end{pmatrix}.$$

$$\tilde{\underline{b}} = \begin{pmatrix} 8.888 \\ -0.5288 \\ 0.7089 \\ 2.55099 \end{pmatrix} - \begin{pmatrix} 0.7617 \\ -0.5288 \\ 0 \\ -0.063 \end{pmatrix}.$$

Now, $SS(E)_{reduced} = (\underline{y} - X\tilde{\underline{b}})^T(\underline{y} - X\tilde{\underline{b}})$.

5. Calculate $\widetilde{\underline{b}}$ for the reduced model $b_2 = 0$. Compare $\widehat{\underline{b}}$ for the full model. What do you see and why?

6. Calculate the non-centralities of Q_1 and Q_2 of Problem 3 as explicit functions of the parameters. The non-centrality of Q is $\frac{1}{2\sigma^2}(X\underline{b})^TA_{H_1}(X\underline{b})$. $Q = \underline{y}^TA_{H_1}\underline{y} = E(\underline{y}^T)A_{H_1}^T\ E(\underline{y}) = \frac{1}{2\sigma^2}\ (K_1^T\underline{b})^T (K_1^T(X^TX)^{-1}K_1)^{-1}(K_1\underline{b}) = \frac{1}{2\sigma^2}(b_1\ \ b_3)\begin{pmatrix} 10 & 5 \\ 5 & 42 \end{pmatrix}\begin{pmatrix} b_1 \\ b_3 \end{pmatrix} = \frac{1}{2\sigma^2}(10b_1^2 + 10b_1b_3 + 42b_3^2)$. The non-centrality of Q_3 is $\frac{1}{2\sigma^2}(24b_2^2)$.

15.19 Two Elementary Models

15.19.1 The One-Way Classification Model

Suppose we want to find the effect on apple yield of a different fertilizers. We get N trees, and fertilize n_i of them with fertilizer i, $i = 1, 2, ..., a$. $N = \sum_{i=1}^{a} n_i$. At the end of the year, we measure the yield from each tree for which a simple model is $y_{ij} = \mu + \alpha_i + \epsilon_{ij}$, $i = 1, 2, ...a$. y_{ij} is the yield from the j-th tree receiving the i-th fertilizer. μ is the average yield of the trees. α_i is the effect for using fertilizer i. ϵ_{ij} is the random error and is assumed to be $N(0, \sigma^2)$. This is an example of a 1-way classification model

$$
\underline{y}_{N\times 1} = \begin{pmatrix} y_{11} \\ y_{12} \\ \vdots \\ y_{1n_1} \\ y_{21} \\ y_{22} \\ \vdots \\ y_{2n_2} \\ \vdots \\ y_{an_a} \end{pmatrix} \quad \underline{b}_{(a+1)\times 1} = \begin{pmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_a \end{pmatrix} \quad X_{N\times(a+1)} = \left(\begin{array}{ccccccc|l} 1 & 1 & 0 & 0 & 0 & \cdots & 0 & \\ 1 & 1 & 0 & 0 & 0 & \cdots & 0 & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\ 1 & 1 & 0 & 0 & 0 & \cdots & 0 & \uparrow n_1 \text{ rows} \\ 1 & 0 & 1 & 0 & 0 & \cdots & 0 & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\ 1 & 0 & 1 & 0 & 0 & \cdots & 0 & \uparrow n_2 \text{ rows} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\ 1 & 0 & 0 & 0 & 0 & \cdots & 1 & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \\ 1 & 0 & 0 & 0 & 0 & \cdots & 1 & \uparrow n_a \text{ rows} \end{array} \right) \quad \underline{e} = \begin{pmatrix} \epsilon_{11} \\ \epsilon_{12} \\ \vdots \\ \epsilon_{1n_1} \\ \epsilon_{21} \\ \epsilon_{22} \\ \vdots \\ \epsilon_{2n_2} \\ \vdots \\ \epsilon_{an_a} \end{pmatrix}
$$

So, the model is $\underline{y} = X\underline{b} + \underline{e}$ where $\underline{e} \sim N(\underline{0}, \sigma^2 I)$. Let's solve the normal equations. Note that $X = (\underline{j}_N \vdots Diag(\underline{j}_{n_i}))$

$$
X^T X = \begin{pmatrix} \underline{j}_N^T \\ \cdots \\ Diag(\underline{j}_{n_i}^T) \end{pmatrix} (\underline{j}_N \vdots Diag(\underline{j}_{n_i})) = \begin{pmatrix} N & n_1 & n_2 & n_3 & \cdots & n_a \\ n_1 & n_1 & 0 & 0 & \cdots & 0 \\ n_2 & 0 & n_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ n_a & 0 & 0 & 0 & 0 & n_a \end{pmatrix}
$$

Clearly, $r(X^T X) = a = r(X)$. A g-inverse of $X^T X$ is

$$
\begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & n_1^{-1} & 0 & \cdots & 0 \\ 0 & 0 & n_2^{-1} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & n_a^{-1} \end{pmatrix}
$$

Also,

$$
X^T \underline{y} = \begin{pmatrix} y_{\cdot\cdot} \\ y_{1\cdot} \\ y_{2\cdot} \\ \vdots \\ y_{a\cdot} \end{pmatrix}
$$

where $y_{\cdot\cdot} = \sum\sum y_{ij}$, $y_{i\cdot} = \sum_{j=1}^{n_i} y_{ij}$, and $y_{\cdot\cdot} = \sum_{i=1}^{a} y_{i\cdot}$. So, one solution to the normal equations is

$$\underline{b}^0 = GX^T\underline{y} = \begin{pmatrix} 0 \\ \bar{y}_{1\cdot} = \frac{y_{1\cdot}}{n_1} \\ \bar{y}_{2\cdot} = \frac{y_{2\cdot}}{n_2} \\ \vdots \\ \bar{y}_{a\cdot} = \frac{y_{a\cdot}}{n_a} \end{pmatrix}$$

Another approach to find a solution is to use the constraint $\mu^0 = \delta$ to solve the equations. Since μ is not estimable, this is okay. Our equations are

$$\begin{pmatrix} X^TX & C \\ C^T & 0 \end{pmatrix} \begin{pmatrix} \underline{b} \\ \underline{\theta} \end{pmatrix} = \begin{pmatrix} X^T\underline{y} \\ \delta \end{pmatrix}$$

which here is

$$\overbrace{\begin{pmatrix} N & n_1 & n_2 & n_3 & \cdots & n_a & 1 \\ n_1 & n_1 & 0 & 0 & \cdots & 0 & 0 \\ n_2 & 0 & n_2 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ n_a & 0 & 0 & 0 & 0 & n_a & 0 \\ 1 & 0 & 0 & 0 & 0 & & 0 \end{pmatrix}}^{\text{invertible to } (a+2)\times(a+2)} \begin{pmatrix} \mu_1 \\ \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_a \\ \theta \end{pmatrix} = \begin{pmatrix} y_{\cdot\cdot} \\ y_{1\cdot} \\ y_{2\cdot} \\ \vdots \\ y_{a\cdot} \\ \delta \end{pmatrix}$$

where $C^T = (1 \;\; 0 \;\; 0 \cdots \;\; 0)$.

$$\begin{pmatrix} X^TX & C \\ C^T & 0 \end{pmatrix}^{-1} = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & n_1^{-1} & 0 & \cdots & 0 & -1 \\ 0 & 0 & n_2^{-1} & \cdots & 0 & -1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & n_a^{-1} & -1 \\ 1 & -1 & -1 & \cdots & -1 & 0 \end{pmatrix} \Rightarrow \begin{pmatrix} \underline{b}^0 \\ \theta \end{pmatrix} = \begin{pmatrix} \underline{\delta} \\ \bar{y}_{1\cdot} - \delta \\ \bar{y}_{2\cdot} - \delta \\ \vdots \\ \bar{y}_{a\cdot} - \delta \\ 0 \end{pmatrix}$$

i.e.

$$\underline{b}^0 = \begin{pmatrix} \delta \\ \bar{y}_{1\cdot} - \delta \\ \bar{y}_{2\cdot} - \delta \\ \vdots \\ \bar{y}_{a\cdot} - \delta \end{pmatrix}.$$

When $\delta = 0$, this is the same solution found above. Note that the partition of

$$\begin{pmatrix} X^TX & C \\ C^T & 0 \end{pmatrix}^{-1}$$

corresponding to X^TX is a g-inverse of X^TX but it is not necessarily the g-inverse corresponding to the solution found by this method. Let's find the usual sums of squares using the first solution. $SS(R) = \underline{y}^TP_x\underline{y} = \underline{y}^TXGX^T\underline{y} =$

$$(y_{\cdot\cdot}\ \ y_{1\cdot}\ \ y_{2\cdot}\ \ \cdots\ \ y_{a\cdot})\begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & n_1^{-1} & 0 & \cdots & 0 \\ 0 & 0 & n_2^{-1} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & n_a^{-1} \end{pmatrix}\begin{pmatrix} y_{\cdot\cdot} \\ y_{1\cdot} \\ y_{2\cdot} \\ \vdots \\ y_{a\cdot} \end{pmatrix} = \sum_{i=1}^{a}\frac{(y_{i\cdot})^2}{n_i}.$$

$SS(E) = SS(TOT) - SS(R) = \sum_i \sum_j y_{ij}^2 - \sum_{i=1}^a \frac{y_{i\cdot}^2}{n_i}$. When there are a column of 1's in the matrix X $SS(M) = N(\bar{y}_{\cdot\cdot})^2 = \frac{(y_{\cdot\cdot})^2}{N}$. $SS(R)_m = SS(R) - SS(m) = \sum_{i=1}^a \frac{y_{i\cdot}^2}{n_i} - \frac{y_{\cdot\cdot}^2}{N}$. $SS(TOT)_m = \sum\sum y_{ij}^2 - \frac{y_{\cdot\cdot}^2}{N}$.

SS	d.f.
$SS(m) = N(\bar{y}_{\cdot\cdot})^2$	1
$SS(R)_m = \sum_{i=1}^a \frac{y_{i\cdot}^2}{n_i} - \frac{y_{\cdot\cdot}^2}{N}$	$a-1$
$SS(E) = \sum_i \sum_j y_{ij}^2 - \sum_{i=1}^a \frac{y_{i\cdot}^2}{n_i}$	$N-a$
$SS(TOT) = \sum\sum y_{ij}^2 - \frac{y_{\cdot\cdot}^2}{N}$	N

$SS(m)$ tests $\overbrace{\mu + \sum_{i=1}^{a}\frac{n_i\alpha_i}{N}}^{=E(\bar{y}_{\cdot\cdot}} = 0$. $SS(R)_m$ tests $\alpha_1 = \alpha_2 = \cdots = \alpha_a$. $SS(m)$ is the $SS(R)$ for the reduced model $y_{ij} = \mu + \epsilon_{ij}$. $SS(R)_m$ is the increase in $SS(R)$ in fitting the model $y_{ij} = \mu + \alpha_i + \epsilon_{ij}$ over and above $y_{ij} = \mu + \epsilon_{ij}$.

Test #2 will be on Thursday, April 17. It will cover Chapters 3, 5, and 6.

These notes cover Section 6.3 in the text book. New notation: $R(\mu)$ is the reduction in $SS(E)$ for fitting $y_{ij} = \mu + \epsilon_{ij}$ over $y_{ij} = \epsilon_{ij} = SS(m)$. $R(\mu, \alpha)$ equals the reduction in $SS(E)$ for fitting $y_{ij} = \mu + \alpha_i + \epsilon_{ij}$ over the model $y_{ij} = \epsilon_{ij}$. $R(\alpha|\mu) = R(\mu, \alpha) - R(\mu)$.

$$P_x = XGX^T = \left(\underline{j}_N \vdots \text{ diag }(\underline{j}_{n_i})\right)\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & n_1^{-1} & 0 & 0 & 0 \\ 0 & 0 & n_2^{-1} & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & n_a^{-1} \end{pmatrix}\begin{pmatrix} \underline{j}_N \\ \cdots \\ \text{diag }(\underline{j}_{n_i}) \end{pmatrix} =$$

$$\left(\underline{0} \vdots \text{ diag }\left(\frac{1}{N_i}\underline{j}_{n_i}\right)\right)\begin{pmatrix} \underline{j}_N \\ \cdots \\ \text{diag }(\underline{j}_{n_i}) \end{pmatrix} = \text{diag }\left(\frac{1}{n_i}\underline{j}_{n_i}\underline{j}_{n_i}^T\right) > \text{diag }\left(\frac{1}{n_i}J_{n_i\times n_i}\right)$$

Estimable Functions

By inspection of X, a general vector in $\Re(X)$ is $(\sum_{i=1}^a \lambda_i,\ \ \lambda_1, \lambda_2, ..., \lambda_a)\,(\mu, \alpha_1, \alpha_2, ..., \alpha_a)$. Hence, the general form of an estimable function is $(\sum_{i=1}^a \lambda_i)\,\mu + \sum_{i=1}^a \lambda_i\alpha_i$ where the $\lambda_i' s$ are arbitrary. There are two important consequences.

1. α_i is not estimable for any i nor is μ.
2. When comparing a group of parameters, $\sum_{i=1}^a \ell_i\alpha_i$ is estimable iff $\sum_{i=1}^a \ell_i = 0$. This is the contrast in the treatment effects.

$$\underline{b}^0 = \begin{pmatrix} \underline{0} \\ \bar{y}_{1\cdot} \\ \bar{y}_{2\cdot} \\ \vdots \\ \bar{y}_{a\cdot} \end{pmatrix} \text{ is one solution.}$$

An Elementary Contrast

An elementary contrast is a contrast of the form $\alpha_i - \alpha_i'$. For our 1-Way Classification model, $\widehat{\alpha_i - \alpha_i'} = \bar{y}_{i\cdot} - \bar{y}_{i\cdot}'$. Any contrast can be written as a linear combination of elementary contrasts and in general, $\sum_{i=1}^a \ell_i\alpha_i = \sum_{i=1}^a \ell_i\bar{y}_{i\cdot}$ where $\sum_{i=1}^a \ell_i = 0$. $Var\left(\sum_{i=1}^a \widehat{\ell_i\alpha_i}\right) = \underline{q}^T G\underline{q}\sigma^2$ where $\underline{q}^T = (0, \ell_1, \ell_2, ..., \ell_a)$ and G is $(X^TX)^-$.

$$\underline{q}^T G\underline{q}\sigma^2 = (0, \ell_1, \ell_2, ..., \ell_a) \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & n_1^{-1} & 0 & 0 & 0 \\ 0 & 0 & n_2^{-1} & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & n_a^{-1} \end{pmatrix} \begin{pmatrix} 0 \\ \ell_1 \\ \ell_2 \\ \vdots \\ \ell_a \end{pmatrix} \sigma^2 = \sigma^2 \sum_{i=1}^a \frac{\ell_i^2}{n_i}.$$

$Cov\left(\sum_{i=1}^a \widehat{\ell_i\alpha_i}, \sum_{i=1}^a \widehat{k_i\alpha_i}\right) = \sigma^2 \sum_{i=1}^a \frac{\ell_i k_i}{n_i}$. The necessary and sufficient conditions for two linear functions of the $\alpha_i's$ to be estimable and to be estimated independently are $\sum_{i=1}^a \ell_i = 0$, $\sum_{i=1}^a k_i = 0$, and $\sum_{i=1}^a \frac{\ell_i k_i}{n_i} = 0$.

Decomposition of $SS(R)$

$SS(R) = \sum_{i=1}^a n_{i\cdot}(\bar{y}_{i\cdot})^2$. Consider $H_i : \mu + \alpha_i = 0$ i.e. $\underline{k}_i^T\underline{b} = 0$ where $\underline{k}_i^T = (1, 0, 0, ..., \overbrace{1,}^{i-th} ..., 0)$. $\underline{k}_i^T\underline{b}^0 = 0 + \bar{y}_{i\cdot} = \bar{y}_{i\cdot}$. $\underline{k}_i^T G\underline{k}_i = \frac{1}{n_i}$. $\underline{k}_i^T G\underline{k}_i{}' = 0\,(i \neq i')$. $SS_{H_i} = (\underline{k}_i^T\underline{b}^0)^T(\underline{k}_i^T G\underline{k}_i)^{-1}(\underline{k}_i^T\underline{b}^0) = \frac{(\bar{y}_{i\cdot})^2}{\frac{1}{n_i}} = n_i(\bar{y}_{i\cdot})^2$. $SS(R) = \sum_{i=1}^a SS_{H_i}$ is a decomposition of $SS(R)$ into a sums of squares with 1 degree of freedom each. Note that $X\underline{b} = \underline{0}$ iff $\mu + \alpha_i = 0, \forall i$.

Invariance of Estimates

This Section covers the invariance of estimates to the choice of $\underline{b}^0$. Consider the family of solutions

$$\underline{b}^0 = \begin{pmatrix} \delta \\ \bar{y}_{1\cdot} - \delta \\ \bar{y}_{2\cdot} - \delta \\ \vdots \\ \bar{y}_{a\cdot} - \delta \end{pmatrix}$$

for any real δ. Since a general estimable function has the form $\mu(\sum_{i=1}^a \lambda_i) + \sum_{i=1}^a \lambda_i\alpha_i$, its estimate is $\delta(\sum_{i=1}^a \lambda_i) + \sum_{i=1}^a \lambda_i(\bar{y}_{i\cdot} - \delta) = \delta(\sum_{i=1}^a \lambda_i) + \sum_{i=1}^a \lambda_i\bar{y}_{i\cdot} - \delta\sum_{i=1}^a \lambda_i = \sum_{i=1}^a \lambda_i\bar{y}_{i\cdot}$, same for every δ. Consider a non-estimable function, $\sum_{i=1}^a \ell_i\alpha_i$ where $\sum_{i=1}^a \ell_i \neq 0$. If we try to estimate this anyway, we get $\sum_{i=1}^a \widehat{\ell_i\alpha_i} = \sum_{i=1}^a \ell_i(\bar{y}_{i\cdot} - \delta) = \sum_{i=1}^a \ell_i\bar{y}_{i\cdot} - \delta\sum_{i=1}^a \ell_i$ which depends on the choice of solution.

Reparameterizing the Model

The model statement is $y_{ij} = \mu + \alpha_i + \epsilon_{ij}$. Suppose we take $\alpha_i' = \alpha_i - \sum_{i=1}^a \frac{n_i\alpha_i}{N}$ and $\mu' = \mu + \sum_{i=1}^a \frac{n_i\alpha_i}{N}$. Then our model is equivalent to $y_{ij} = \mu' + \alpha_i' + \epsilon_{ij}$ and α_i' satisfies $\sum_{i=1}^a \frac{\alpha_i' n_i}{N} = 0$. Consider

$$\underline{b}_1^0 = \begin{pmatrix} \bar{y}_{\cdot\cdot} \\ \bar{y}_{1\cdot} - \bar{y}_{\cdot\cdot} \\ \vdots \\ \bar{y}_{a\cdot} - \bar{y}_{\cdot\cdot} \end{pmatrix}, \quad E(\underline{b}_1^0) = \begin{pmatrix} \mu + \sum_{i=1}^a \frac{n_i\alpha_i}{N} \\ \alpha_1 - \sum_{i=1}^a \frac{n_i\alpha_i}{N} \\ \alpha_2 - \sum_{i=1}^a \frac{n_i\alpha_i}{N} \\ \vdots \\ \alpha_a - \sum_{i=1}^a \frac{n_i\alpha_i}{N} \end{pmatrix} = \begin{pmatrix} \mu' \\ \alpha_1' \\ \alpha_2' \\ \vdots \\ \alpha_a' \end{pmatrix}.$$

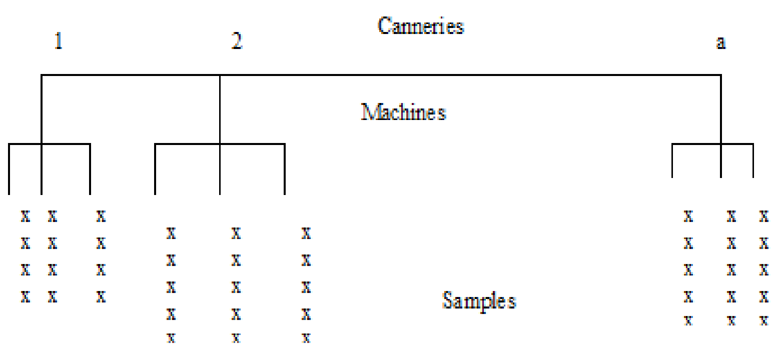
So, every linear function of

$$\underline{b}_1 = \begin{pmatrix} \mu' \\ \alpha_1' \\ \alpha_2' \\ \vdots \\ \alpha_a' \end{pmatrix} \text{ is estimable.}$$

But α_i' is not especially meaningful where $\alpha_i' = \alpha_i - \sum_{i=1}^a \frac{n_i\alpha_i}{N}$.

15.19.2 Two-Way Nested Classification

Example: We send several hundred bushels of our apples to each of a local canneries. Cannery i produces cans of apple sauce with each of their b_i saucing machines. We have n_{ij} samples evaluated for purity of the apple sauce from machine j in cannery i. Let y_{ijk} be the purity measure of sample k from machine j in cannery i. The model statement is $y_{ijk} = \mu + \alpha_i + \beta_{ij} + \epsilon_{ijk}$, $i = 1, 2, ..., a$; $j = 1, 2, ..., b_i$; $k = 1, 2, ..., n_{ij}$. α_i is the cannery effect. β_{ij} is the effect of machine j in cannery i. ϵ_{ijk} is the random error. The machines are nested. They can not be in two canneries.



$$\underline{b} = \begin{pmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_a \\ \beta_{11} \\ \beta_{12} \\ \vdots \\ \beta_{1n_1} \\ \beta_{21} \\ \beta_{22} \\ \vdots \\ \beta_{2n_2} \\ \vdots \\ \beta_{a1} \\ \vdots \\ \beta_{an_a} \end{pmatrix}, \quad \underline{y} = \begin{pmatrix} y_{111} \\ y_{112} \\ \vdots \\ y_{11n_1} \\ y_{121} \\ y_{122} \\ \vdots \\ y_{12n_2} \\ \vdots \\ y_{ab_a1} \\ y_{ab_a2} \\ \vdots \\ y_{ab_an_a} \end{pmatrix}$$

$N = n_{\cdot\cdot} = \sum_{i=1}^{a}\sum_{j=1}^{b_i} n_{ij}$. Let $b. = \sum_{i=1}^{a} b_i$, $n_{i\cdot} = \sum_{j=1}^{b_i} n_{ij}$.

$$X = \left\{ \underline{j}_N \vdots \, diag(\underline{j}_{n_{i\cdot}}) \vdots \, diag(\underline{j}_{n_{ij}}) \right\}$$

$$X^T X = \begin{pmatrix} \underline{j}_N^T \\ \cdots \\ diag(\underline{j}_{n_{j\cdot}}^T) \\ \cdots \\ diag(\underline{j}_{n_{ij}}^T) \end{pmatrix} \left(\underline{j}_N \vdots \, diag(\underline{j}_{n_{i\cdot}}) \vdots \, diag(\underline{j}_{n_{ij}}) \right) =$$

$$\begin{array}{c|cccccc|cccc}
N & n_{1\cdot} & n_{2\cdot} & n_{3\cdot} & \cdots & n_{a\cdot} & & n_{11} & n_{12} & \cdots & n_{ab_a} \\
\hline
n_{1\cdot} & n_{1\cdot} & & & & & & & & & \\
n_{2\cdot} & & n_{2\cdot} & & 0 & & & & diag(\underline{n}_i^T) & & \\
\vdots & & 0 & & & & & & & & \\
n_{a\cdot} & & & & & n_{a\cdot} & & & & & \\
\hline
n_{11} & & & & & & & n_{11} & & & \\
n_{12} & & & & & & & & n_{12} & & 0 \\
\vdots & & & diag(\underline{n}_i^T) & & & & & & & \\
n_{ab_a} & & & & & & & & 0 & & n_{ab_a}
\end{array}$$

where $n_{i\cdot}^T = (n_{i1} \;\; n_{i2} \;\; \cdots n_{ib_i})$, $r(X^T X) = b. = \sum_{i=1}^{a} b_i = r(X)$. A g-inverse of $X^T X$ is

$$G = \begin{array}{c} \overbrace{\quad 1 \quad a \quad\quad\quad b. \quad}^{} \\ \left(\begin{array}{c|ccc|c} 1 & 0 & & 0 & 0 \\ --- & --- & & --- & --- \\ a & 0 & & 0 & 0 \\ --- & --- & & --- & --- \\ b\cdot & 0 & & 0 & diag(n_{ij}^{-1}) \end{array}\right) \end{array} \qquad X^T\underline{y} = \left(\begin{array}{c} y_{\ldots} \\ --- \\ y_{1\cdot\cdot} \\ y_{2\cdot\cdot} \\ \vdots \\ y_{a\cdot\cdot} \\ --- \\ y_{11\cdot} \\ y_{112\cdot} \\ \vdots \\ y_{ab_a a.} \end{array}\right) \begin{array}{l} 1 \\ \\ a \\ \\ \\ b. \end{array}$$

The solution is

$$\underline{b}^0 = GX^T\underline{y} = \left(\begin{array}{c} 0 \\ --- \\ \underline{0}_a \\ --- \\ \bar{y}_{11\cdot} \\ \bar{y}_{12\cdot} \\ \vdots \\ \bar{y}_{ab_{ab_a}.} \end{array}\right)$$

$SS(R) = \underline{y}^T P_x \underline{y} = \underline{y}^T XGX^T \underline{y} = (X^T\underline{y})^T \underline{b}^0 = \sum_{i=1}^{a}\sum_{j=1}^{b_i} y_{ij\cdot}\bar{y}_{ij\cdot} = \sum_{i=1}^{a}\sum_{j=1}^{b_i} \frac{(y_{ij\cdot})^2}{n_{ij}}$. $SS(TOTAL) = \sum_i^a \sum_j^{b_i} \sum_k^{n_{ij}} y_{ijk}^2$. Then, $SS(E) = SS(TOTAL) - SS(R) = \sum_i\sum_j\sum_k y_{ijk}^2 - \sum_i\sum_j \frac{(y_{ij\cdot})^2}{n_{ij}}$. $SS(M) = N(\bar{y}_{\ldots})^2$. $SS(R)_m = SS(R) - SS(M)$.

Source	d.f.	SS
Mean	1	$SS(M) = N(\bar{y}_{\ldots})^2$
Model (a.f.m)	$b. - 1$	$SS(R)_m = \sum_i\sum_j \frac{(y_{ij\cdot})^2}{n_{ij}} - N(\bar{y}_{\ldots})^2$
Error	$N - b.$	$SS(E) = \sum_i\sum_j\sum_k y_{ijk}^2 - \sum_i\sum_j \frac{(y_{ij\cdot})^2}{n_{ij}}$
Total	N	$SS(TOTAL) = \sum_i\sum_j\sum_k y_{ijk}^2$

Suppose we just fit the model $y_{ijk} = \mu + \alpha_i + \epsilon_{ijk}$. For this model $SS(R) = R(\mu,\alpha) = \sum_{i=1}^{a} \frac{y_{i\cdot\cdot}^2}{n_{i\cdot}}$. For the full model, the reduction in $SS(E)$ is $R(\mu,\alpha,\beta) = \sum_i\sum_j \frac{(y_{ij\cdot})^2}{n_{ij}}$. Therefore, the change in $SS(E)$ from the smaller model with just $\alpha_i' s$ to the full model is $R(\beta|\mu,\alpha) = R(\mu,\alpha,\beta) - R(\mu,\alpha)$. Also, $R(\mu) = N(\bar{y}_{\ldots})^2$. So, $R(\alpha|\mu) = R(\mu,\alpha) - R(\mu)$.

Source	d.f.	SS
Mean	1	$R(\mu)$
Canneries (after machines)	$a - 1$	$R(\alpha\|\mu)$
Machines (after canneries)	$b. - a$	$R(\beta\|\mu,\alpha)$
Error	$N - b.$	$SS(E)$
Total	N	$SS(TOTAL)$

$R(\beta|\mu,\alpha)$ is used to test the hypothesis $H : \beta_{i1} = \beta_{i2} = \cdots = \beta_{ib_i}$, $i = 1,2,...,a$. $R(\alpha|\mu)$ is used to test the hypothesis $H_0 : \alpha_i + \sum_j \frac{n_{ij}\beta_{ij}}{n_{i\cdot}}$ being equal for $i = 1,2,...,a$.

Estimable Functions (Nested)

The model statement is $y_{ijk} = \mu + \alpha_i + \beta_{ij} + \epsilon_{ijk}$. The list of estimable functions is

1. $\mu + \alpha_i + \beta_{ij}$, $i = 1, 2, ..., a$; $j = 1, 2, ..., b_i$. This is the full set of LIN estimable functions.
2. Contrasts in the $\beta_{ij}'s$ for fixed i. That is, $\sum_{j=1}^{b_i} w_i \beta_{ij}$ where $\sum_{j=1}^{b_i} w_j = 0$.
3. Generalizing (2), $\sum_{i=1}^{a} \ell_i \sum_{j=1}^{b_i} w_{ij}\beta_{ij}$ where $\sum_{j=1}^{b_i} w_{ij} = 0$, $i = 1, 2, ..., a$.
4. $\sum_{i=1}^{a} \ell_i\alpha_i + \sum_{i=1}^{a} \ell_i \sum_{j=1}^{b_i} w_{ij}\beta_{ij}$ where $\sum_{j=1}^{b_i} w_{ij} = 1$ for $i = 1, 2, ..., a$ and $\sum_{i=1}^{a} \ell_i = 0$. A special case of this is when $w_{ij} = \frac{1}{b_i}$, to get $\sum_{i=1}^{a} \ell_i\alpha_i + \sum_{i=1}^{a} \ell_i\bar{\beta}_{i\cdot} = \sum_{i=1}^{a} \ell_i(\alpha_i + \bar{\beta}_{i\cdot})$.
5. Contrasts in the $\alpha_i's$ are not estimable and no individual parameter is estimable.

	B.L.U.E.S.	Variances
(1)	$\bar{y}_{ij\cdot}$	σ^2/n_{ij}
(2)	$\sum_{j=1}^{b_i} w_j \bar{y}_{ij\cdot}$	$\sigma^2 \sum_{j=1}^{b_i} \frac{w_j^2}{n_{ij}}$
(3)	$\sum_{i=1}^{a} \ell_i \sum_{j=1}^{b_i} w_{ij}\bar{y}_{ij\cdot}$	$\sigma^2 \sum_{i=1}^{a} \ell_i^2 \sum_{j=1}^{b_i} \frac{w_{ij}^2}{n_{ij}}$

15.20 Homework and Answers

In the text book on page 225, work Problem 9. You simply need to show that the Q is the same for both hypotheses.

9. $Q_1 = (\lambda K^T\underline{b} - \underline{m})^T(\lambda K^T G\lambda K)^{-1}(\lambda K^T\underline{b} - \underline{m})$ where G is a g-inverse of X^TX. $Q_1 = (\lambda K^T\underline{b})^T \frac{(K^TGK)^{-1}}{\lambda\lambda}(\lambda K^T\underline{b}) = (K^T\underline{b})^T(K^TGK)^{-1}(K^T\underline{b})$. $Q_2 = (K^T\underline{b} - \underline{m})^T(K^TGK)^{-1}(K^T\underline{b} - \underline{m}) = (K^T\underline{b})^T(K^TGK)^{-1}(K^T\underline{b}) \Rightarrow Q_1 = Q_2$. Testing $\lambda K^T\underline{b} = \underline{0}$ is the same as testing $K^T\underline{b} = \underline{0}$.

1. In a preliminary experiment to compare the effects of three drug regiments on rat brain mass, two rats were assigned to each of the three regiments. It was intended that all six rats have the same parents, but discovered after the fact that two of them had a different mother. An appropriate model for the six observations thus obtained is

$$\begin{aligned}
y_1 &= \mu + \alpha_1 + \beta_1 + e_1\\
y_2 &= \mu + \alpha_1 + \beta_1 + e_2\\
y_3 &= \mu + \alpha_2 + \beta_1 + e_3\\
y_4 &= \mu + \alpha_3 + \beta_1 + e_4\\
y_5 &= \mu + \alpha_2 + \beta_2 + e_5\\
y_6 &= \mu + \alpha_3 + \beta_2 + e_6
\end{aligned}$$

where α_i is the effect of drug regimen i, β_j is the effect of mother j, and the $e's$ are iid $N(0, \sigma^2)$. The observation vector is $\underline{y} = (94,\ 99,\ 83,\ 88,\ 80,\ 76)'$.

(a) Write down the model in matrix notation. Find a solution to the normal equations by finding a generalized inverse of $X'X$. $\underline{y} = X\underline{b} + \underline{e}$ where

$$\underline{y} = \begin{pmatrix} 94\\ 99\\ 83\\ 88\\ 80\\ 76 \end{pmatrix}, \quad X = \begin{pmatrix} \mu & \alpha_1 & \alpha_2 & \alpha_3 & \beta_1 & \beta_2\\ \hline 1 & 1 & 0 & 0 & 1 & 0\\ 1 & 1 & 0 & 0 & 1 & 0\\ 1 & 0 & 1 & 0 & 1 & 0\\ 1 & 0 & 0 & 1 & 1 & 0\\ 1 & 0 & 1 & 0 & 0 & 1\\ 1 & 0 & 0 & 1 & 0 & 1 \end{pmatrix}, \quad \underline{b} = \begin{pmatrix} \mu\\ \alpha_1\\ \alpha_2\\ \alpha_3\\ \beta_1\\ \beta_2 \end{pmatrix}.$$

$$X^T X = \begin{pmatrix} 6 & 2 & 2 & 2 & 4 & 2 \\ 2 & 2 & 0 & 0 & 2 & 0 \\ 2 & 0 & 2 & 0 & 1 & 1 \\ 2 & 0 & 0 & 2 & 1 & 1 \\ 4 & 2 & 1 & 1 & 4 & 0 \\ 2 & 0 & 1 & 1 & 0 & 2 \end{pmatrix}$$

Find a sub-matrix of $X^T X$ to make a g-inverse.

$$G = \begin{pmatrix} \frac{3}{4} & -\frac{1}{4} & -\frac{1}{2} & 0 & -\frac{1}{2} & 0 \\ -\frac{1}{4} & \frac{5}{4} & \frac{1}{2} & 0 & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$GX^T = \begin{pmatrix} 0 & 0 & -0.25 & 0.25 & 0.25 & 0.75 \\ 0.50 & 0.50 & -0.25 & -0.75 & 0.25 & -0.25 \\ 0 & 0 & 0.50 & -0.50 & 0.50 & -0.50 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.50 & 0.50 & -0.50 & -0.50 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

$$GX^T \underline{y} = \begin{pmatrix} 78.25 \\ 10.75 \\ -0.50 \\ 0 \\ 7.50 \\ 0 \end{pmatrix} = \underline{b}^0.$$

(b) Show that $\alpha_1 - \alpha_2$ and $\alpha_2 - \alpha_3$ are estimable. Interpret these linear functions in terms of the experiment. $\underline{q}^T = (0,\ 1,\ -1,\ 0,\ 0,\ 0)$. Let

$$H = G(X^T X) = \begin{pmatrix} 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

$\underline{q}^T H = (0,\ 1,\ -1,\ 0,\ 0,\ 0) = \underline{q}^T \Rightarrow \underline{q}^T$ is estimable. $\alpha_1 - \alpha_2$ is the difference in effects of drugs 1 and 2 on brain mass. For the second part, $\underline{q}^T = (0,\ 0,\ 1,\ -1,\ 0,\ 0)$. Then, $\underline{q}^T H = (0,\ 0,\ 1,\ -1,\ 0,\ 0) = \underline{q}^T \Rightarrow \underline{q}^T$ is estimable. $\alpha_2 - \alpha_3$ is the difference of the effects of drugs 2 and 3 on brain mass.

(c) Find $r(X)$ linearly independent estimable functions including $\alpha_1 - \alpha_2$ and $\alpha_2 - \alpha_3$. It is known that $\alpha_1 - \alpha_2$ and $\alpha_2 - \alpha_3$ are estimable. For $\underline{q}^T = \mu + \alpha_1 - \beta_2$, $\underline{q}^T = (1,\ 1,\ 0,\ 0,\ 0,\ -1)$. $\underline{q}^T H = (1,\ 1,\ 0,\ 0,\ 0,\ -1) \Rightarrow \mu + \alpha_1 - \beta_2$ is estimable. For $\mu + \alpha_2 - \alpha_3 + \beta_2$, $\underline{q}^T = (1,\ 0,\ 1,\ -1,\ 0,\ 1)$. $\underline{q}^T H = (1,\ 0,\ 1,\ 0,\ 0,\ 1) \neq \underline{q}^T \Rightarrow \mu + \alpha_2 - \alpha_3 + \beta_2$ is not estimable. For $\mu + \alpha_2 + \beta_2$, $\underline{q}^T = (1,\ 0,\ 1,\ 0,\ 0,\ 1)$. $\underline{q}^T H = (1,\ 0,\ 1,\ 0,\ 0,\ 1) \Rightarrow \mu + \alpha_2 + \beta_2$ is estimable. Since $r(X) = 4$, cannot have 5 linearly independent estimable functions.

(d) Show that $\mu, \alpha_1, \alpha_2, \alpha_3, \beta_1$, and β_2 are not estimable. For μ, $\underline{q}^T = (1,\ 0,\ 0,\ 0,\ 0,\ 0)$. $\underline{q}^T H = (1,\ 0,\ 0,\ 1,\ 0,\ 1) \neq \underline{q}^T \Rightarrow \mu$ is not estimable. For α_1, $\underline{q}^T = (0,\ 1,\ 0,\ 0,\ 0,\ 0)$. $\underline{q}^T H = (0,\ 1,\ 0,\ -1,\ 0,\ 0) \neq \underline{q}^T \Rightarrow \alpha_1$ is not estimable. For α_2, $\underline{q}^T = (0,\ 0,\ 1,\ 0,\ 0,\ 0)$. $\underline{q}^T H = (0,\ 0,\ 1,\ -1,\ 0,\ 0) \neq \underline{q}^T \Rightarrow \alpha_2$ is not estimable. For α_3, $\underline{q}^T = (0,\ 0,\ 0,\ 1,\ 0,\ 0)$. $\underline{q}^T H = (0,\ 0,\ 0,\ 0,\ 0,\ 0) \neq \underline{q}^T \Rightarrow \alpha_3$ is not estimable. For β_1, $\underline{q}^T = (0,\ 0,\ 0,\ 0,\ 1,\ 0)$. $\underline{q}^T H = (-4,\ 0,\ 0,\ 0,\ 1,\ -1) \neq \underline{q}^T \Rightarrow \beta_1$ is not estimable. For β_2, $\underline{q}^T = (0,\ 0,\ 0,\ 0,\ 0,\ 1)$. $\underline{q}^T H = (0,\ 0,\ 0,\ 0,\ 0,\ 0) \neq \underline{q}^T \Rightarrow \beta_2$ is not estimable.

(e) Test the two hypotheses $H_1 : \alpha_1 = \alpha_2 = \alpha_3$ and $H_2 : \beta_1 = \beta_2$. Are the $Q's$ for testing these two hypotheses independent? Why or why not? Calculate the non-centralities of the two quadratic forms as explicit functions of the parameters. For $H_1 : \alpha_1 = \alpha_2 = \alpha_3$,

$$K^T = \begin{pmatrix} 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \end{pmatrix}, \ \underline{m} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

$$K^T G = \begin{pmatrix} 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \frac{3}{4} & -\frac{1}{4} & -\frac{1}{2} & 0 & -\frac{1}{2} & 0 \\ -\frac{1}{4} & \frac{5}{4} & \frac{1}{2} & 0 & -\frac{1}{2} & 0 \\ -\frac{1}{2} & \frac{1}{2} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} =$$

$$\begin{pmatrix} 0.25 & 0.75 & -0.50 & 0.00 & -0.50 & 0.00 \\ -0.50 & 0.50 & 1.00 & 0.00 & 0.00 & 0.00 \end{pmatrix}$$

$$K^T G K = \begin{pmatrix} 0.25 & 0.75 & -0.50 & 0.00 & -0.50 & 0.00 \\ -0.50 & 0.50 & 1.00 & 0.00 & 0.00 & 0.00 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ -1 & 1 \\ 0 & -1 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1.25 & -0.50 \\ -0.50 & 1.00 \end{pmatrix}.$$

Find $(K^T G K)^{-1}$ to get.

$$(K^T G K)^{-1} = \begin{pmatrix} 1.00 & 0.50 \\ 0.50 & 1.25 \end{pmatrix}.$$

$$K^T \underline{b}^0 - \underline{m} = \begin{pmatrix} 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 78.25 \\ 10.75 \\ -0.50 \\ 0 \\ 7.5 \\ 0 \end{pmatrix} = \begin{pmatrix} 11.25 \\ -0.50 \end{pmatrix}.$$

$$(K^T\underline{b}^0 - \underline{m})^T(K^TGK)^{-1} = (11.25,\ \ -0.50)\begin{pmatrix} 1.00 & 0.50 \\ 0.50 & 1.25 \end{pmatrix} = (11,\ \ 5).$$

$$(K^T\underline{b}^0 - \underline{m})^T(K^TGK)^{-1}(K^T\underline{b}^0 - \underline{m}) = (11,\ \ 5)\begin{pmatrix} 11.25 \\ -0.50 \end{pmatrix} = 121.25 = Q_1.$$

$SS(T) = \underline{y}^T\underline{y} = 45446.$

$$\widehat{\underline{y}} = \begin{pmatrix} 96.5 \\ 96.5 \\ 85.25 \\ 85.75 \\ 77.75 \\ 78.25 \end{pmatrix},$$

$Q_1 = SS(E)_{reduced} - SS(E)_{full} \Rightarrow SS(E)_{full} = 32.75.$

$$F = \frac{121.25/2}{32.75/(6-4)} = 3.70$$

Find $F_{0.05}(2,2)$ for the cut-off. Now, for the hypothesis $H_2 : \beta_1 = \beta_2$, $K^T = (0,\ \ 0,\ \ 0,\ \ 0,\ \ 1,\ \ -1)$. $\underline{m} = 0$. $K^TG = \left(-\frac{1}{2},\ \ -\frac{1}{2},\ \ 0,\ \ 0,\ \ 1,\ \ 0\right)$.

$$K^TGK = \left(-\frac{1}{2},\ \ -\frac{1}{2},\ \ 0,\ \ 0,\ \ 1,\ \ 0\right)\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ -1 \end{pmatrix} = 1 \Rightarrow (K^TGK)^{-1} = 1.$$

$$(K^T\underline{b}^0 - \underline{m}) = (0,\ \ 0,\ \ 0,\ \ 0,\ \ 1,\ \ -1)\begin{pmatrix} 78.25 \\ 10.75 \\ -0.50 \\ 0 \\ 7.5 \\ 0 \end{pmatrix} = 7.5.$$

$(K^T\underline{b}^0 - \underline{m})^T(K^TGK)^{-1}(K^T\underline{b}^0 - \underline{m}) = 7.5(1)(7.5) = 56.25$. $F = \frac{56.25/1}{32.75/(6-1)}$. Is $K_1^T(X^TX)^{-}K_2 = 0$?

$$K_1^TGK_2 = \begin{pmatrix} 0.25 & 0.75 & -0.50 & 0.00 & -0.50 & 0.00 \\ -0.50 & 0.50 & 1.00 & 0.00 & 0.00 & 0.00 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ -1 \end{pmatrix} = \begin{pmatrix} -0.5 \\ 0.0 \end{pmatrix} \neq \underline{0}$$

$\Rightarrow Q_1$ and Q_2 are dependent.

The non-centrality of Q_1 is

$$\frac{1}{2\sigma^2}(K_1^T\underline{b})^T(K_1^T(X^TX)^-K_1)^{-1}(K_1\underline{b}) = \frac{1}{2\sigma^2}(\alpha_1-\alpha_2,\ \ \alpha_2-\alpha_3)\begin{pmatrix} 1.00 & 0.50 \\ 0.50 & 1.25 \end{pmatrix}\begin{pmatrix} \alpha_1-\alpha_2 \\ \alpha_2-\alpha_3 \end{pmatrix}$$

or, for independence $SS(R) = SS(T) - SS(E) = 45446 - 32.75 = 45413.25$. $SSR(M) = SS(R) - SS(M) = 45413.25 - 45066.67 = 346.58$. Does $Q_1 + Q_2 = 346.58$? $177.5 \neq 346.58 \Rightarrow$ dependent. The non-centrality for H_1 is

$$\frac{1}{2\sigma^2}(\alpha_1-\alpha_2,\ \ \alpha_2-\alpha_3)\begin{pmatrix} 1.25 & 0.50 \\ 0.50 & 1.00 \end{pmatrix}\begin{pmatrix} \alpha_1-\alpha_2 \\ \alpha_2-\alpha_3 \end{pmatrix} =$$

$$\frac{1}{2\sigma^2}(1.25(\alpha_1-\alpha_3) - 0.5(\alpha_2-\alpha_3),\ \ -0.5(\alpha_1-\alpha_2)+(\alpha_2-\alpha_3))\begin{pmatrix} \alpha_1-\alpha_2 \\ \alpha_2-\alpha_3 \end{pmatrix}$$

$$= \frac{1}{2\sigma^2}\left[(1.25(\alpha_1-\alpha_2) - 0.5(\alpha_2-\alpha_3))(\alpha_1-\alpha_2) + (-0.5(\alpha_1-\alpha_2)+(\alpha_2-\alpha_3))(\alpha_2-\alpha_3)\right].$$

The non-centrality for H_2 is

$$\frac{1}{2\sigma^2}(\beta_1-\beta_2)(1)(\beta_1-\beta_2) = \frac{1}{2\sigma^2}(\beta_1-\beta_2)^2.$$

(f) What is the reduced model corresponding to H_2? Write down a full set of linearly independent estimable functions for this reduced model — do it sot that they are orthogonal to one another. $\underline{y} = X\underline{b} + \underline{e}$ where

$$\underline{y} = \begin{pmatrix} 94 \\ 99 \\ 83 \\ 88 \\ 80 \\ 76 \end{pmatrix}, \quad X = \begin{pmatrix} \mu & \alpha_1 & \alpha_2 & \alpha_3 \\ \hline 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{pmatrix}.$$

The rank of X is $r(X) = 3$. $\mu+\alpha_1$, $\mu+\alpha_2$, and $\mu+\alpha_3$.

(g) Consider the reduced model corresponding to the hypothesis H_2 in (e). What is $SSR(M)$ for this model? What is the hypothesis for this $SSR(M)$? Test that hypothesis.

(h) Suppose both rats receiving additive #3 had mother #2, but the other four had mother #1. Are the functions you listed in (c) still estimable? Find a full set of linearly independent estimable functions for this situation.

$$X = \begin{pmatrix} \mu & \alpha_1 & \alpha_2 & \alpha_3 & \beta_1 & \beta_2 \\ \hline 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 \end{pmatrix}$$

$$G = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 \\ -\frac{1}{2} & 1 & \frac{1}{2} & 0 & 0 & 0 \\ -\frac{1}{2} & \frac{1}{2} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

$$H = G(X^T X) = \begin{pmatrix} 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & -1 & 1 & -1 \\ 0 & 0 & 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Is $\alpha_1 - \alpha_2$ still estimable? $\underline{q}^T = (0,\ 1,\ -1,\ 0,\ 0,\ 0)$. $\underline{q}^T H = (0,\ 1,\ -1,\ 0,\ 0,\ 0) = \underline{q}^T \Rightarrow \alpha_1 - \alpha_2$ is still estimable. Is $\alpha_2 - \alpha_3$ still estimable? $\underline{q}^T = (0,\ 0,\ 1,\ -1,\ 0,\ 0)$. $\underline{q}^T H = (0,\ 0,\ 1,\ -1,\ 1,\ -1) \neq \underline{q}^T \Rightarrow \alpha_2 - \alpha_3$ is not estimable. Is $\mu + \alpha_1 - \beta_2$ still estimable? $\underline{q}^T = (1,\ 1,\ 0,\ 0,\ 0,\ -1)$. $\underline{q}^T H = (1,\ 1,\ 0,\ 0,\ 1,\ 0) \neq \underline{q}^T \Rightarrow \mu + \alpha_1 - \beta_2$ is not estimable. Is $\mu + \alpha_2 - \alpha_3 + \beta_2$ still estimable? $\underline{q}^T = (1,\ 0,\ 1,\ -1,\ 0,\ 1)$. $\underline{q}^T H = (1,\ 0,\ 1,\ 0,\ 1,\ 0) \neq \underline{q}^T \Rightarrow \mu + \alpha_2 - \alpha_3 + \beta_2$ is not estimable. Is $\mu + \alpha_2 + \beta_2$ still estimable? $\underline{q}^T = (1,\ 0,\ 1,\ 0,\ 0,\ 1)$. $\underline{q}^T H = (1,\ 0,\ 1,\ 0,\ 1,\ 0) \neq \underline{q}^T \Rightarrow \mu + \alpha_2 + \beta_2$ is not estimable. Is $\alpha_1 - \alpha_3 + \beta_1 - \beta_2$ still estimable? $\underline{q}^T = (0,\ 1,\ 0,\ -1,\ 1,\ -1)$. $\underline{q}^T H = (0,\ 1,\ 0,\ -1,\ 1,\ -1) = \underline{q}^T \Rightarrow \alpha_1 - \alpha_3 + \beta_1 - \beta_2$ is estimable. Is $\mu + \alpha_3 + \beta_2$ still estimable? $\underline{q}^T = (1,\ 0,\ 0,\ 1,\ 0,\ 1)$. $\underline{q}^T H = (1,\ 0,\ 0,\ 1,\ 0,\ 1) = \underline{q}^T \Rightarrow \mu + \alpha_3 + \beta_2$ is estimable.

2. At the start of Chapter 5 in the text book, for the general linear model with $Var(\underline{y}) = V$ and not assuming X has full column rank, we found the normal equations $X'V^{-1}X\underline{b} = X'V^{-1}\underline{y}$. Prove that these equations are consistent. Need to show that $X^T V^{-1}\underline{y} \in \varrho(X^T V^{-1} X) = \Re(X^T V^{-1} X) = \Re(X^T X) = \Re(X)$. $X^T V^{-1}\underline{y} = X^T \underline{w}$ where $\underline{w} = V^{-1}\underline{y}$. $X^T \underline{w} \in \varrho(X^T) = \Re(X)$. You can not use the g-inverse of $X^T X$ because this assumes consistency.

15.21 Two-Way Crossed Classification Design

This Section covers Chapter 7 in the text book. We have two factors: factor 1 at a levels and factor 2 at b levels. Each measurement is on an experimental unit which will receive one of the levels of factor 1 and one of the levels of factor 2. n_{ij} is the number of observations with level i of factor 1 and level j of factor 2.

15.21.1 Without Interaction

This section covers Section 7.1 in the text book. The model is $y_{ijk} = \mu + \alpha_i + \beta_j + \epsilon_{ijk}$, $i = 1, ..., a$; $j = 1, ..., b$; $k = 1, ..., n_{ij}$. $N = n_{..} = \sum_i \sum_j n_{ij}$. To express this in vector notation,

$$\underline{b}_{(a+b+1)\times 1} = \begin{pmatrix} \mu \\ \underline{\alpha} \\ \underline{\beta} \end{pmatrix} \text{ where } \underline{\alpha} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_a \end{pmatrix} \text{ and } \underline{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_b \end{pmatrix}.$$

Define the matrices $A_{N\times a}$, $L_{N\times b}$, and $N_{a\times b}$ as

$$(A)_{r,s} = \begin{cases} 1, & \text{if } r\text{-th obs receives } \alpha_s. \\ 0, & \text{otherwise.} \end{cases}$$

$$(L)_{r,s} = \begin{cases} 1, & \text{if } r\text{-th obs receives } \beta_s. \\ 0, & \text{otherwise.} \end{cases}$$

$(N)_{r,s} = n_{r,s}$ e.g. the different sample sizes. Now the model can be written $\underline{y} = \mu \underline{j}_N + A\underline{\alpha} + L\underline{\beta} + \underline{e} = X\underline{b} + \underline{e}$ where $X = (\underline{j}_N \vdots A \vdots L)$. Some useful facts include.

1. $\underline{j}_N^T A = (n_{1\cdot} \;\; n_{2\cdot} \;\; \cdots n_{a\cdot})_{1\times a}$
2. $\underline{j}_N^T L = (n_{\cdot 1} \;\; n_{\cdot 2} \;\; \cdots n_{\cdot b})_{1\times b}$
3. $A\underline{j}_a = \underline{j}_N$
4. $L\underline{j}_b = \underline{j}_N$
5. $A^T A = D(n_{i\cdot})_{a\times a}$
6. $L^T L = D(n_{\cdot j})_{b\times b}$
7. $(A^T L)_{a\times b} = N$
8. $A^T \underline{y} = \underline{y}_a$
9. $L^T \underline{y} = \underline{y}_b$

where

$$\underline{y}_a = \begin{pmatrix} y_{1\cdot\cdot} \\ y_{2\cdot\cdot} \\ \vdots \\ y_{a\cdot\cdot} \end{pmatrix}, \; \underline{y}_b = \begin{pmatrix} y_{\cdot 1\cdot} \\ y_{\cdot 2\cdot} \\ \vdots \\ y_{\cdot b\cdot} \end{pmatrix}, \; \underline{\bar{y}}_a = \begin{pmatrix} \bar{y}_{1\cdot\cdot} \\ \bar{y}_{2\cdot\cdot} \\ \vdots \\ \bar{y}_{a\cdot\cdot} \end{pmatrix} = D(n_{i\cdot})^{-1}\underline{y}_a = (A^T A)^{-1}A^T\underline{y},$$

and

$$\underline{\bar{y}}_b = \begin{pmatrix} \bar{y}_{\cdot 1\cdot} \\ \bar{y}_{\cdot 2\cdot} \\ \vdots \\ \bar{y}_{\cdot b\cdot} \end{pmatrix} = D^{-1}(n_{\cdot j})\underline{y}_b = (L^T L)^{-1}L^T\underline{y}.$$

The normal equations are

$$X^T X = \begin{pmatrix} \underline{j}_N^T \\ A^T \\ L^T \end{pmatrix} (\underline{j}_N \;\; A \;\; L) = \begin{pmatrix} \underline{j}_N \underline{j}_N & \underline{j}_N^T A & \underline{j}_N^T L \\ A^T \underline{j}_N & A^T A & A^T L \\ L^T \underline{j}_N & L^T A & L^T L \end{pmatrix} =$$

$$\left(\begin{array}{c|cccc|cccc} N & n_{1\cdot} & n_{2\cdot} & \cdots & n_{a\cdot} & n_{\cdot 1} & n_{\cdot 2} & \cdots & n_{\cdot b} \\ \hline n_{1\cdot} & & & & & & & & \\ n_{2\cdot} & & & & & & & & \\ n_{i\cdot} & & D(n_{i\cdot}) & & & & N & & \\ n_{a\cdot} & & & & & & & & \\ \hline n_{\cdot 1} & & & & & & & & \\ n_{\cdot 2} & & & & & & & & \\ n_{\cdot j} & & N^T & & & & D(n_{\cdot j}) & & \\ n_{\cdot b} & & & & & & & & \end{array}\right)$$

Note that the a columns $n_{1\cdot}, n_{2\cdot}, ..., n_{a\cdot}$ sum to 1 and the b columns $n_{\cdot 1}, n_{\cdot 2}, ..., n_{\cdot b}$ sum to 1. The rank $r(X) = r(X^TX) \leq a+b-1$. The solution to the normal equations is

$$X^T\underline{y} = \begin{pmatrix} \underline{j}_N^T \\ A^T \\ L^T \end{pmatrix} \underline{y} = \begin{pmatrix} y_{\cdots} \\ \underline{y}_a \\ \underline{y}_b \end{pmatrix}.$$

So, the normal equations are $X^TX\underline{b} = X^T\underline{y}$, $N\mu + \sum_{i=1}^a n_{i\cdot}\alpha_i + \sum_{j=1}^b n_{\cdot j}\beta_j = y_{\cdots}$, $A^T\underline{j}_N\mu + D(n_{i\cdot})\underline{\alpha} + N\underline{\beta} = \underline{y}_a$, $L^T\underline{j}_N\mu + N^T\underline{\alpha} + D(n_{\cdot j})\underline{\beta} = \underline{y}_b$. So, we have three equations. First note that μ is not estimable. Hence, we can impose the non-estimable constraint $\mu^0 = 0$. This yields

1. $D(n_{i\cdot})\underline{\alpha}^0 + N\underline{\beta}^0 = \underline{y}_a$
2. $N^T\underline{\alpha}^0 + D(n_{\cdot j})\underline{\beta}^0 = \underline{y}_b$

From (1) we get:

$\underline{\alpha}^0 = D(n_{i\cdot})^{-1}[\underline{y}_a - N\underline{\beta}^0] \Rightarrow N^T[D(n_{i\cdot})^{-1}[\underline{y}_a - N\underline{\beta}^0]] + D(n_{\cdot j})\underline{\beta}^0 = \underline{y}_b \Rightarrow \overbrace{(D(n_{\cdot j}) - N^TD^{-1}(n_{i\cdot})N)}^{\text{call it } F}\underline{\beta}^0 = \underline{y}_b - N^TD(n_{i\cdot}^{-1})\underline{y}_a$. We have $F\underline{\beta}^0 = \underline{y}_b - N^T\underline{\bar{y}}_a$. Solving by letting $\Im$ be a g-inverse of F. $\underline{\beta}^0 = \Im(\underline{y}_b - N^T\underline{\bar{y}}_a)$, $\underline{\alpha}^0 = \underline{\bar{y}}_a - D^{-1}(n_{i\cdot})N\Im(\underline{y}_b - N^T\underline{\bar{y}}_a)$, and $\underline{\mu}^0 = 0$. The g-inverse of X^TX corresponding to this solution is

$$G = \begin{pmatrix} 0 & \underline{0}_a^T & \underline{0}_b^T \\ \underline{0}_a & [I + D^{-1}(n_{i\cdot})N\Im N^T]D(n_{i\cdot}^{-1}) & -D(n_{i\cdot}^{-1})N\Im \\ \underline{0}_b & -\Im N^TD(n_{i\cdot}^{-1}) & \Im \end{pmatrix}$$

Example: See page 261 of the text book. $a = 4, b = 3, N = 9$.

$$A_{9\times 4} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad L_{9\times 3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \underline{y}_{9\times 1} = \begin{pmatrix} 18 \\ 12 \\ 24 \\ 9 \\ 3 \\ 15 \\ 6 \\ 3 \\ 18 \end{pmatrix}.$$

$$N_{4\times 3} = (n_{ij}) = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix} = A^T L.$$

Note that $A\underline{j}_4 = L\underline{j}_3 = \underline{j}_N$. $\underline{j}_N^T A = (3,\ 1,\ 2,\ 3) = (n_{1\cdot},\ n_{2\cdot},\ n_{3\cdot},\ n_{4\cdot})$. $\underline{j}_N^T L = (3,\ 2,\ 4) = (n_{\cdot 1},\ n_{\cdot 2},\ n_{\cdot 3})$.

$$A^T A = \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix} = D(n_{i\cdot}),\quad L^T L = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{pmatrix} = D(n_{\cdot j}).$$

$$A^T \underline{y} = \begin{pmatrix} 54 \\ 9 \\ 18 \\ 27 \end{pmatrix} = \underline{y}_a,\quad \underline{\bar{y}}_a = D(n_{i\cdot}^{-1})\underline{y}_a = \begin{pmatrix} 18 \\ 9 \\ 9 \\ 9 \end{pmatrix}.$$

$$L^T \underline{y} = \begin{pmatrix} 27 \\ 15 \\ 66 \end{pmatrix} = \underline{y}_b,\quad \underline{\bar{y}}_b = D(n_{\cdot j}^{-1})\underline{y}_b = \begin{pmatrix} 9 \\ 7.5 \\ 16.5 \end{pmatrix}.$$

$$F = D(n_{\cdot j}) - N^T D(n_{i\cdot}^{-1})N = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{3} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix} =$$

$$\begin{pmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{pmatrix} - \frac{1}{6}\begin{pmatrix} 7 & 4 & 7 \\ 4 & 4 & 4 \\ 7 & 4 & 13 \end{pmatrix} = \frac{1}{6}\begin{pmatrix} 11 & -4 & -7 \\ -4 & 8 & -4 \\ -7 & -4 & 11 \end{pmatrix}.$$

A g-inverse of F is

$$\Im = \frac{1}{12}\begin{pmatrix} 8 & 4 & 0 \\ 4 & 11 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

$R(\mu) = \frac{1}{N} = \underline{y}^T J \underline{y} = \frac{1}{N}(y_{\cdot\cdot\cdot})^2 = \frac{1}{9}(108)^2 = 1296$. $R(\underline{\alpha}|\mu) = \underline{\bar{y}}_a^T D(n_{i\cdot})\underline{\bar{y}}_a - \frac{1}{N}\underline{y}^T J \underline{y} = \sum_{i=1}^a n_{i\cdot}(\bar{y}_{i\cdot})^2 - \frac{1}{N}(y_{\cdot\cdot\cdot})^2 = 1458 - 1296 = 162$.

$$R(\underline{\beta}|\mu, \underline{\alpha}) = (\underline{y}_b - N^T \underline{\bar{y}}_a)^T \Im (\underline{y}_b - N^T \underline{\bar{y}}_a) =$$

$$(-9,\ -12,\ 21)\frac{1}{12}\begin{pmatrix} 8 & 4 & 0 \\ 4 & 11 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} -9 \\ -12 \\ 21 \end{pmatrix} = 258.$$

$r(\underline{\alpha}|\mu, \underline{\beta}) = R(\mu, \underline{\alpha}, \underline{\beta}) - R(\mu, \underline{\beta}) = R(\underline{\beta}|\mu, \underline{\alpha}) + R(\underline{\alpha}|\mu) + R(\mu) - R(\mu, \underline{\beta}) = 258 + 162 + 1296 - \underline{y}_b^T D(n_{\cdot j}^{-1})\underline{y}_b = 1716 - 1444.5 = 271.5$. $R(\underline{\beta}|\mu) = R(\mu, \underline{\beta}) - R(\mu) = 1444.5 - 1296 = 148.5$. The ANOVA tables are on page 272 of the text book. Solve for the normal equations.

$\underline{\beta}^0 = \Im(\underline{y}_b - N^T \underline{\bar{y}}_a)$.

$$\underline{y}_b - N^T \underline{\bar{y}}_a = \begin{pmatrix} 27 \\ 15 \\ 66 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 18 \\ 9 \\ 9 \\ 9 \end{pmatrix} = \begin{pmatrix} -9 \\ -12 \\ 21 \end{pmatrix} \Rightarrow$$

$$\underline{\beta}^0 = \frac{1}{12} \begin{pmatrix} 8 & 4 & 0 \\ 4 & 11 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} -9 \\ -12 \\ 21 \end{pmatrix} = \begin{pmatrix} -10 \\ -14 \\ 0 \end{pmatrix}.$$

$$\underline{\alpha}^0 = \underline{\bar{y}}_a - D(n_{i\cdot}^{-1}) N \underline{\beta}^0 = \begin{pmatrix} 18 \\ 9 \\ 9 \\ 9 \end{pmatrix} - \begin{pmatrix} \frac{1}{3} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} -10 \\ -14 \\ 0 \end{pmatrix} = \begin{pmatrix} 26 \\ 9 \\ 14 \\ 17 \end{pmatrix}.$$

A solution to the normal equations is $\underline{b}^0 = (0,\ 26,\ 9,\ 14,\ 17,\ -10,\ -14,\ 0)^T$.

Summary

The model is $\underline{y} = \mu \underline{j}_N + A\underline{\alpha} + L\underline{\beta} + \underline{e} = X\underline{b} + \underline{e}$ where $X = (\underline{j}_N \ \ A \ \ L)$ and $\underline{b}^T = (\mu \ \ \underline{\alpha} \ \ \underline{\beta})$. In the last class, we solved the normal equations and found $\underline{\beta}^0 = \Im(\underline{y}_b - N^T \underline{\bar{y}}_a)$, $\underline{\alpha}^0 = \underline{\bar{y}}_a - D(n_{i\cdot}^{-1}) N \Im(\underline{y}_b - N^T \underline{\bar{y}}_a)$, and $\mu^0 = 0$. Here are some notes on this solution and this method of approach.

1. If all of the $n_{ij} > 0$, or more generally, if the rank $r(F) = b - 1$, then writing F_{b-1} for the upper $(b-1) \times (b-1)$ diagonal sub-matrix of F
   (a) F_{b-1} is non-singular.
   (b) $\Im = \begin{pmatrix} F_{b-1}^{-1} & \underline{0}_{b-1} \\ \underline{0}_{b-1}^T & 0 \end{pmatrix}$ is a g-inverse of F.
   (c) We can use this g-inverse $\Im$ to solve the normal equations corresponding to the restriction $\beta_b^0 = 0$.
2. Our method above of solving the normal equations is called "absorbing the $\alpha' s$ into the $\beta' s$" since we eliminated $\underline{\alpha}$ from the equations and solved explicitly for $\underline{\beta}^0$.
3. Likewise, starting with (1) and (2), we could absorb the $\beta' s$ into the $\alpha' s$ by eliminating $\underline{\beta}$ and solving for $\underline{\alpha}^0$.

Let's find the H matrix for absorbing the $\alpha' s$.

$$H_\alpha = \begin{pmatrix} 0 & \underline{0}_a^T & \underline{0}_b^T \\ \underline{0}_a & [I + D(n_{i\cdot}^{-1}) N \Im N^T] D(n_{i\cdot}^{-1}) & -D(n_{i\cdot}^{-1}) N \Im \\ \underline{0}_b & -\Im N^T D(n_{i\cdot}^{-1}) & \Im \end{pmatrix} \begin{pmatrix} \underline{j}_N^T \underline{j}_N & \underline{j}_N^T A & \underline{j}_N^T L \\ A^T \underline{j}_N & A^T A & A^T L \\ L^T \underline{j}_N & L^T A & L^T L \end{pmatrix} =$$

$$\begin{pmatrix} 0 & \underline{0}_a^T & \underline{0}_b^T \\ \underline{j}_a & I_a & D(n_{i\cdot}^{-1})[I - \Im F] \\ \underline{0}_b & 0_{b \times a} & \Im F \end{pmatrix}$$

The intermediate calculations are as follow: for cell (2,1) $[I + D(n_{i.}^{-1})N\Im N^T]\overbrace{D(n_{i.}^{-1})A^T\underline{j}_N}^{\underline{j}_a} - D(n_{i.}^{-1})N\Im \overbrace{L^T\underline{j}_N}^{N^T\underline{j}_a} = \underline{j}_a$. For cell (2,2): $[I + D(n_{i.}^{-1})N\Im N^T]\overbrace{D(n_{i.}^{-1})D(n_{i.})}^{=I} - D(n_{i.}^{-1})N\Im N^T = I_a$. For cell (2,3): $[I + D(n_{i.}^{-1})N\Im N^T]A^T L - D(n_{i.}^{-1})N\Im L^T L = [I + D(n_{i.}^{-1})N\Im N^T]N - D(n_{i.}^{-1})N\Im D(n_{.j}) = D(n_{i.}^{-1})N - D(n_{i.}^{-1})N\Im \overbrace{[D(n_{.j}) - N^T D(n_{i.}^{-1})N]}^{=F} = D(n_{i.}^{-1})N - D(n_{i.}^{-1})N\Im F = D(n_{i.}^{-1})[I - \Im F]$. For cell (3,1): $-\Im N^T\overbrace{D(n_{i.}^{-1})A^T\underline{j}_N}^{\underline{j}_a} + \Im L^T\underline{j}_N = -\Im L^T\overbrace{A\underline{j}_a}^{\underline{j}_N} + \Im L^T\underline{j}_N = \underline{0}_b$. For cell (3,2): $-\Im N^T D(n_{i.}^{-1})A^T A + \Im L^T A = -\Im N^T D(n_{i.}^{-1})D(n_{i.}) + \Im N^T = 0_{b\times a}$. For cell (3,3): $-\Im N^T D(n_{i.}^{-1})N + \Im L^T L = -\Im N^T D(n_{i.}^{-1})N + \Im D(n_{.j}) = \Im\overbrace{[D(n_{.j}) - N^T D(n_{i.}^{-1})N]}^{=F} = \Im F$.

ANOVA Tables

In the ANOVA Table, $SS(R) = R(\mu,\alpha,\beta) = \underline{b}^{0^T}X^T\underline{y} = (\underline{\mu}^0\ \underline{\alpha}^{0^T}\ \underline{\alpha}^{0^T})\begin{pmatrix}\underline{j}_N^T\underline{y}\\ \underline{y}_a\\ \underline{y}_b\end{pmatrix} = \underline{\alpha}_0^T\underline{y}_a + \underline{\beta}_0^T\underline{y}_b = (\underline{\bar{y}}_a - D(n_{i.}^{-1})N\underline{\beta}_0)^T\underline{y}_a + \underline{\beta}_0^T\underline{y}_b = \underline{\bar{b}}_a\underline{y}_a + \underline{\beta}_0^T[\underline{y}_b - N^T D(n_{i.}^{-1})\underline{y}_a] = \underline{y}_a^T D(n_{i.}^{-1})\underline{y}_a + (\underline{y}_b - N^T\underline{\bar{y}}_a)^T\Im(\underline{y}_b - N^T\underline{\bar{y}}_a)$. As usual, $SS(M) = R(\mu) = \frac{1}{N}\underline{y}^T J_N\underline{y}$ and from Chapter 6 in the text book, $R(\mu,\alpha) = \sum_{i=1}^a \frac{y_{i..}^2}{n_{i.}} = \underline{y}_a^T D(n_{i.}^{-1})\underline{y}_a \Rightarrow R(\alpha|\mu) = R(\mu,\alpha) - R(\mu) = \underline{y}_a^T D(n_{i.}^{-1})\underline{y}_a - \frac{1}{N}\underline{y}^T J_N\underline{y} = \underline{y}^T[A\,D(n_{i.}^{-1})\,A^T - \frac{1}{N}J_N]\underline{y}$. $R(\beta|\mu,\alpha) = R(\mu,\alpha,\beta) - R(\mu,\alpha) = (\underline{y}_b - N^T\underline{\bar{y}}_a)^T\Im(\underline{y}_b - N^T\underline{\bar{y}}_a)$. The breakdown gives the following ANOVA table.

Source	SS	d.f.
μ	$SS(M) = \frac{1}{N}\underline{y}^T J_N\underline{y}$	1
$\alpha's$ after μ	$R(\alpha\|\mu) = \underline{y}^T[A\,D(n_{i.}^{-1})\,A^T - \frac{1}{N}J_N]\underline{y}$	$a-1$
$\beta's$ after μ and α	$R(\beta\|\mu,\alpha) = (\underline{y}_b - N^T\underline{\bar{y}}_a)^T\Im(\underline{y}_b - N^T\underline{\bar{y}}_a)$	$b-1$
Error	$SS(E) = SS(T) - R(\mu,\alpha,\beta) = \sum_{i=1}^N y_i^2 - \underline{b}^{0^T}X^T\underline{y}$	$N-a-b+1$
Total	$SS(T) = \sum_{i=1}^N y_i^2$	

It is very important that the rank of X $r(x) = a+b-1$ for the degrees of freedom of $R(\beta|\mu,\alpha)$ to be $b-1$. We can put an emphasis on the $\alpha's$ by letting the $\beta's$ absorb into the $\alpha's$. We will need to find $R(\beta|\mu)$ and $R(\alpha|\mu,\beta)$. The ANOVA table is as follow.

Source	SS	d.f.
μ	$R(\mu) = \frac{1}{N}\underline{y}^T J_N\underline{y}$	1
$\beta's$ after μ	$R(\beta\|\mu) = \underline{y}_b^T D(n_{.j}^{-1})\underline{y}_b - \frac{1}{N}\underline{y}^T J_N\underline{y}$	$b-1$
$\alpha's$ after μ and β	$R(\alpha\|\mu,\beta) = (\underline{y}_a - N\underline{\bar{y}}_b)^T\varrho(\underline{y}_a - N\underline{\bar{y}}_b)$	$a-1$
Error	$SS(E)$	$N-a-b+1$
Total	$SS(T)$	N

where $R(\beta|\mu) = \underline{y}_b^T D(n_{.j}^{-1})\underline{y}_b - \frac{1}{N}\underline{y}^T J_N\underline{y}$ and $R(\alpha|\mu,\beta) = (\underline{y}_a - N\underline{\bar{y}}_b)^T\varrho(\underline{y}_a - N\underline{\bar{y}}_b)$ where ϱ is a g-inverse of

$C = D(n_{i\cdot}) - ND(n_{\cdot j}^{-1})N^T$.

15.22 Homework and Answers

1. Text book page 259, Problem 1. The model is $y_{ij} = \mu_i + \epsilon_{ij}$ where y_{ij} is the j^{th} observation on the i^{th} treatment, μ_i is the mean of the i^{th} treatment, and ϵ_{ij} is random error. Let $i = 1, 2, ..., a$ and $j = 1, 2, ..., n_i$. $N = \sum_{i=1}^{a} n_i$.

$$X_{N\times a} = \begin{array}{c} \begin{array}{ccccc} \mu_1 & \mu_2 & \mu_3 & \cdots & \mu_a \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & & 0 \\ 1 & 0 & 0 & & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & 0 & 0 & & 0 \\ 0 & 1 & 0 & & 0 \\ 0 & 1 & 0 & & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 1 & 0 & & 0 \\ 0 & 0 & 1 & & 0 \\ 0 & 0 & 1 & & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 1 & & 0 \\ 0 & 0 & 0 & & 0 \\ 0 & 0 & 0 & & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & & 0 \\ 0 & 0 & 0 & & 1 \\ 0 & 0 & 0 & & 1 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & & 1 \end{pmatrix} \end{array}, \quad \underline{b}_{a\times 1} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \\ \vdots \\ \mu_a \end{pmatrix}, \quad \underline{y}_{N\times 1} = \begin{pmatrix} y_{11} \\ y_{12} \\ \vdots \\ y_{1n_1} \\ y_{21} \\ y_{22} \\ \vdots \\ y_{2n_2} \\ \vdots \\ y_{a1} \\ y_{a2} \\ \vdots \\ y_{an_a} \end{pmatrix}.$$

Note that X can be rewritten as

$$X = \begin{pmatrix} \underline{j}_{n_1} & 0 & 0 & 0 & 0 \\ 0 & \underline{j}_{n_2} & 0 & 0 & 0 \\ 0 & 0 & \underline{j}_{n_3} & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \underline{j}_{n_a} \end{pmatrix}$$

$(X^TX)^{-1}X^TX = I_{a\times a}$. Suppose $\underline{K}^T = (1,\ 0,\ 0, \cdots, 0,\ 0)$ which corresponds to μ_1. Then $\underline{K}^T$ $(X^TX)^{-1}\ X^TX = \underline{K}^T \Rightarrow$ estimable. For each $\mu_i, i = 1, 2, ..., a$ is going to be estimable with a similar argument. To find the B.L.U.E., $\underline{b}^0 = GX^TV^{-1}\underline{y}$ is a solution to the normal equations $(X^TV^{-1}X)\underline{b} = X^TV^{-1}\underline{y}$ where G is a g-inverse of $X^TV^{-1}X$. By Theorem 5.1, $\underline{q}^T\underline{b}^0$ is the B.L.U.E. of $\underline{q}^T\underline{b}$ where $\underline{q}^T \in \Re(X)$. So, use $\underline{q}^T\widehat{\underline{b}} = \bar{y}_{i\cdot}$.

2. Text book page 260, Problem 11 parts (a)-(d). Use PROC GLM in SAS for parts (a)-(c) and indicate on your listing the answers to each question. In (b), make the table adjusted for the mean. For (c), although SAS prints these two tests by default, I want you to also test them using the CONTRAST statement. Be careful, (ii) is tricky. For (d), just do (i). You do not actually have to run the test — just show that the required property holds true. If there is anything that you don't know how to do in SAS, please see me.

```
data survey;
input course $ section y @@;
cards;
e 1 2 e 1 5 e 1 2 e 2 7 e 2 9 e 3 8 e 3 4 e 3 3 e 3 6 e 3 4
g 1 2 g 1 6 g 2 10 g 2 8 g 2 9
c 1 8 c 2 6 c 2 2 c 2 3 c 2 1 c 3 1 c 3 3 c 3 2 c 4 8 c 4 6
;
run;

proc glm order = data;
  class course section;
  model y = course section(course)/xpx i solution;
  contrast 'sections' section(course) 1 -1 0 0 0 0 0 0 0,
                      section(course) 1 0 -1 0 0 0 0 0 0,
                      section(course) 0 0 0 1 -1 0 0 0 0,
  section(course) 0 0 0 0 0 1 -1 0 0,
  section(course) 0 0 0 0 0 0 1 -1 0,
  section(course) 0 0 0 0 0 0 0 1 -1;
  contrast 'courses'
    course 1 -1 0 section(course) .3 .2 .5 -.4 -.6 0 0 0 0,
course 1 0 -1 section(course) .3 .2 .5 0 0 -.1 -.4 -.3 -.2;
run;
```

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                    The SAS System                    15:42 Sunday, August 31, 2008  17

                   The GLM Procedure

                Class Level Information

            Class         Levels    Values

            course             3    e g c

            section            4    1 2 3 4


        Number of Observations Read          25
        Number of Observations Used          25
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                    The SAS System                    15:42 Sunday, August 31, 2008  18

                   The GLM Procedure

             Matrix Element Representation

                 Dependent Variable: y

        Effect                   Representation

        Intercept                Intercept

        course             e     course e
        course             g     course g
        course             c     course c

        section(course)    1 e   Dummy001
        section(course)    2 e   Dummy002
        section(course)    3 e   Dummy003
        section(course)    1 g   Dummy004
        section(course)    2 g   Dummy005
        section(course)    1 c   Dummy006
        section(course)    2 c   Dummy007
        section(course)    3 c   Dummy008
        section(course)    4 c   Dummy009
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                    The SAS System                    15:42 Sunday, August 31, 2008  19

                   The GLM Procedure
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The X'X Matrix

	Intercept	course e	course g	course c	Dummy001	Dummy002	Dummy003
Intercept	25	10	5	10	3	2	5
course e	10	10	0	0	3	2	5
course g	5	0	5	0	0	0	0
course c	10	0	0	10	0	0	0
Dummy001	3	3	0	0	3	0	0
Dummy002	2	2	0	0	0	2	0
Dummy003	5	5	0	0	0	0	5
Dummy004	2	0	2	0	0	0	0
Dummy005	3	0	3	0	0	0	0
Dummy006	1	0	0	1	0	0	0
Dummy007	4	0	0	4	0	0	0
Dummy008	3	0	0	3	0	0	0
Dummy009	2	0	0	2	0	0	0
y	125	50	35	40	9	16	25

The X'X Matrix

	Dummy004	Dummy005	Dummy006	Dummy007	Dummy008	Dummy009	y
Intercept	2	3	1	4	3	2	125
course e	0	0	0	0	0	0	50
course g	2	3	0	0	0	0	35
course c	0	0	1	4	3	2	40
Dummy001	0	0	0	0	0	0	9
Dummy002	0	0	0	0	0	0	16
Dummy003	0	0	0	0	0	0	25
Dummy004	2	0	0	0	0	0	8
Dummy005	0	3	0	0	0	0	27
Dummy006	0	0	1	0	0	0	8
Dummy007	0	0	0	4	0	0	12
Dummy008	0	0	0	0	3	0	6
Dummy009	0	0	0	0	0	2	14

y	8	27	8	12	6	14	817

The SAS System 15:42 Sunday, August 31, 2008 20

The GLM Procedure

X'X Generalized Inverse (g2)

	Intercept	course e	course g	course c	Dummy001	Dummy002	Dummy003
Intercept	0.5	-0.5	-0.5	0	-2.06563E-18	-3.57634E-17	0
course e	-0.5	0.7	0.5	0	-0.2	-0.2	0
course g	-0.5	0.5	0.8333333333	0	9.817827E-18	4.541712E-17	0
course c	0	0	0	0	0	0	0
Dummy001	-2.06563E-18	-0.2	9.817827E-18	0	0.5333333333	0.2	0
Dummy002	-3.57634E-17	-0.2	4.541712E-17	0	0.2	0.7	0
Dummy003	0	0	0	0	0	0	0
Dummy004	9.637541E-17	-7.41755E-17	-0.333333333	0	-6.88935E-18	-8.16969E-18	0
Dummy005	0	0	0	0	0	0	0
Dummy006	-0.5	0.5	0.5	0	2.928475E-18	3.724743E-17	0
Dummy007	-0.5	0.5	0.5	0	2.928475E-18	3.724743E-17	0
Dummy008	-0.5	0.5	0.5	0	7.557266E-18	3.956062E-17	0
Dummy009	0	0	0	0	0	0	0
y	7	-2	2	0	-2	3	0

X'X Generalized Inverse (g2)

	Dummy004	Dummy005	Dummy006	Dummy007	Dummy008	Dummy009	y
Intercept	9.637541E-17	0	-0.5	-0.5	-0.5	0	7
course e	-7.41755E-17	0	0.5	0.5	0.5	0	-2
course g	-0.333333333	0	0.5	0.5	0.5	0	2
course c	0	0	0	0	0	0	0
Dummy001	-6.88935E-18	0	2.928475E-18	2.928475E-18	7.557266E-18	0	-2
Dummy002	-8.16969E-18	0	3.724743E-17	3.724743E-17	3.956062E-17	0	3
Dummy003	0	0	0	0	0	0	0
Dummy004	0.8333333333	0	-9.63754E-17	-9.63754E-17	-9.38042E-17	0	-5
Dummy005	0	0	0	0	0	0	0
Dummy006	-9.63754E-17	0	1.5	0.5	0.5	0	1
Dummy007	-9.63754E-17	0	0.5	0.75	0.5	0	-4
Dummy008	-9.38042E-17	0	0.5	0.5	0.8333333333	0	-5
Dummy009	0	0	0	0	0	0	0
y	-5	0	1	-4	-5	0	52

The SAS System 15:42 Sunday, August 31, 2008 21

The GLM Procedure

Dependent Variable: y

Source	DF	Sum of Squares	Mean Square	F Value	Pr > F
Model	8	140.0000000	17.5000000	5.38	0.0021
Error	16	52.0000000	3.2500000		
Corrected Total	24	192.0000000			

R-Square	Coeff Var	Root MSE	y Mean
0.729167	36.05551	1.802776	5.000000

Source	DF	Type I SS	Mean Square	F Value	Pr > F
course	2	30.0000000	15.0000000	4.62	0.0262
section(course)	6	110.0000000	18.3333333	5.64	0.0026

Source	DF	Type III SS	Mean Square	F Value	Pr > F
course	2	6.9505298	3.4752649	1.07	0.3665
section(course)	6	110.0000000	18.3333333	5.64	0.0026

Contrast	DF	Contrast SS	Mean Square	F Value	Pr > F
sections	6	110.0000000	18.3333333	5.64	0.0026
courses	2	30.0000000	15.0000000	4.62	0.0262

The SAS System 15:42 Sunday, August 31, 2008 22

The GLM Procedure

Dependent Variable: y

Parameter		Estimate	Standard Error	t Value	Pr > |t|
Intercept		7.000000000 B	1.27475488	5.49	<.0001
course	e	-2.000000000 B	1.50831031	-1.33	0.2035
course	g	2.000000000 B	1.64570147	1.22	0.2419
course	c	0.000000000 B	.	.	.
section(course)	1 e	-2.000000000 B	1.31656118	-1.52	0.1482
section(course)	2 e	3.000000000 B	1.50831031	1.99	0.0641
section(course)	3 e	0.000000000 B	.	.	.
section(course)	1 g	-5.000000000 B	1.64570147	-3.04	0.0078
section(course)	2 g	0.000000000 B	.	.	.
section(course)	1 c	1.000000000 B	2.20794022	0.45	0.6567
section(course)	2 c	-4.000000000 B	1.56124950	-2.56	0.0209
section(course)	3 c	-5.000000000 B	1.64570147	-3.04	0.0078
section(course)	4 c	0.000000000 B	.	.	.

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NOTE: The X'X matrix has been found to be singular, and a generalized inverse was used to solve the normal equations.  Terms whose
      estimates are followed by the letter 'B' are not uniquely estimable.
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For H_1 : sections within courses have the same opinions,

$$K^T = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \end{pmatrix}.$$

For H_2 : courses have similar opinions,

$$K^T = \begin{pmatrix} 0 & 1 & -1 & 0 & \frac{3}{10} & \frac{2}{10} & \frac{5}{10} & -\frac{2}{5} & -\frac{3}{5} & 0 & 0 & 0 & 0 \\ \\ 0 & 1 & 0 & -1 & \frac{3}{10} & \frac{2}{10} & \frac{5}{10} & 0 & 0 & -\frac{1}{10} & -\frac{4}{10} & -\frac{3}{10} & -\frac{2}{10} \end{pmatrix}$$

3. Do the following.

   (a) Let D be an $n \times n$ diagonal matrix with no zeros on the diagonal. For a given x such that $D+xJ$ is non-singular, find y so that $(D+xJ)^{-1} = D^{-1} + yD^{-1}JD^{-1}$.

   (b) For the 1-way classification model, consider the hypothesis $H_0 : K'\underline{b} = \underline{0}$ where $K' = (\underline{0}_{a-1} \mid \underline{j}_{a-1} \mid - I_{a-1})$.

      i. Write down H_0 in terms of $\mu, \alpha_1, ..., \alpha_a$. $(D+XJ)^{-1} = D^{-1}+YD^{-1}JD^{-1}$. $(D+XJ)(D^{-1}+YD^{-1}JD^{-1}) = I$. $I+YJD^{-1}+XJD^{-1}+XYJD^{-1}JD^{-1} = I$. $YJD^{-1}+XJD^{-1}+XYJD^{-1}JD^{-1} = 0$. Post-multiply by D. $YJ+XJ+XYJD^{-1}J = 0$. $(X+Y)J+XYtr(D^{-1})J = 0$. $(X+Y+XYtr(D^{-1}))J = 0$. Solve $X+Y+XYtr(D^{-1}) = 0$. $Y = \frac{-X}{1+X\,tr(D^{-1})} = -\frac{1}{\frac{1}{X}+tr(D^{-1})}$.

      ii. Show that the sum of squares for testing H_0 is $\sum_{i=1}^{a} n_i(\bar{y}_{i\cdot})^2 - N(\bar{y}_{\cdot\cdot})^2$ by showing that $K'GK = \frac{1}{n_1}J_{a-1} + D^{i\neq 1}(n_i^{-1})$ and using the result in (a) to find $(K'GK)^{-1}$. Here $D^{i\neq 1}(n_i^{-1})$ is $(a-1)\times(a-1)$ with $n_2^{-1}, ..., n_a^{-1}$ on the diagonal.

      iii. What is the non-centrality?

15.23 Test and Answers

Everyone must work problems 1 and 2. Then work two problems from among 3, 4, and 5. Work carefully and use your time wisely. The model used throughout is $\underline{y} = X\underline{b} + \underline{\epsilon}$ where $\underline{\epsilon} \sim N(\underline{0}, \sigma^2 I)$. Do not assume that X has full column rank unless stated in a particular problem.

1. (15 points) Do the following.

   (a) State completely the theorem for testing a general linear hypothesis $K'\underline{b} = \underline{m}$, including conditions on K' and th complete distribution of the test statistic.

   (b) Let W be a non-singular matrix with dimension equal to the number of rows in K' of (a). Prove that the hypothesis $H_0 : WK'\underline{b} = \underline{0}$ is testable. Then prove that the test statistic for this H_0 is identical to that for $H_0 : K'\underline{b} = \underline{0}$. $H_0 : \overbrace{WK^T}^{=K_1^T}\underline{b} = 0$. To get the test statistic, you must get the same degrees of freedom. So, show the rank $r(K_1^T) = r(K^T)$ i.e $r(WK^T) = r(K^T)$ which is true since W is non-singular. Also, $K_1^T\underline{b} = \underline{0}$ is testable since $K_1^T = WK^T$ and $\Re(K^T) \subseteq \Re(X) \Rightarrow K^T = SX$. Therefore, $K_1^T = WSX \Rightarrow \Re(K_1^T) = \Re(K^T)$. Now just show K_1^T gives the same Q as K^T. $(K_1^T\underline{b}^0)^T(K_1^TGK_1)^{-1}(K_1^T\underline{b}^0) = (WK^T\underline{b}^0)^T(WK^TGKW^T)^{-1}(WK^T\underline{b}^0) = (K^T\underline{b}^0)^TW^T(W^T)^{-1}(K^TGK)^{-1}W^{-1}W(K^T\underline{b}^0) = (K^T\underline{b}^0)^T\ (K^TGK)^{-1}(K^T\underline{b}^0) = Q$ for testing $H_0 : K^T\underline{b} = \underline{0}$.

2. (15 points) Six measurements are available, for which

$$\begin{aligned} E(y_1) &= \mu + \alpha_1 \\ E(y_2) &= \mu + \alpha_1 + \beta_1 \\ E(y_3) &= \mu + \alpha_2 + \beta_1 \\ E(y_4) &= \mu + \alpha_1 + \beta_1 \\ E(y_5) &= \mu + \beta_2 + \beta_2 \\ E(y_6) &= \mu + \alpha_2 + \beta_1 \end{aligned}$$

With $\underline{b} = (\mu, \alpha_1, \alpha_2, \beta_1, \beta_2)'$, a generalized inverse of $X'X$ is

$$\begin{pmatrix} 1 & -1 & -1 & 0 & 1 & -1 \\ -1 & 2 & 2 & -1 & 1 & -1 \\ -1 & 2 & 3 & -1.5 & 1 & -1 \\ 0 & -1 & -1.5 & 1.5 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -1 & -1 \end{pmatrix}.$$

The data vector is $\underline{y} = (0,\ 5,\ 6,\ 7,\ 2,\ 8)'$ and $SS(E) = 4$.

(a) Show that $\alpha_1 - \alpha_2$ and β_1 are estimable.

(b) Find the rank $r(X)$ linearly independent estimable functions including $\alpha_1 - \alpha_2$ and β_1.

(c) Write in a simple fashion the hypothesis tested by $SSR(M)$. Do not test the hypothesis. $H_0 :$ $\mu + \alpha_1 = \mu + \alpha_1 + \beta_1 = \mu + \alpha_2 + \beta_1 = \mu + \beta_2 + \gamma$ or $H_0 : \beta_1 = 0,\ \mu + \alpha_1 = \mu + \alpha_2 = \mu + \beta_2 + \gamma$ or $H_0 : \beta_1 = 0,\ \alpha_1 = \alpha_2, \alpha_2 = \beta_2 + \gamma$. $SS(R)_m$ tests that each observation has the same expected value.

$$K^T = \begin{pmatrix} 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

(d) Test the hypothesis $\alpha_1 - \alpha_2, \beta_1 = 0$.

(e) What is the reduced model corresponding to the hypothesis in (d)? What does $SSR(M)$ for that model test? Do not test the hypothesis.

i	$E(y_i)$
1	$\mu + \alpha_1$
2	$\mu + \alpha_1$
3	$\mu + \alpha_1$
4	$\mu + \alpha_1$
5	$\mu + \beta_2 + \gamma$
6	$\mu + \alpha_1$

$SS(R)_m$ for this model tests $H_0 : \alpha_1 = \beta_2 + \gamma$.

3. (10 points) Do the following.

(a) State the normal equations.

(b) Prove that the normal equations are consistent, and then give a solution $\underline{b}^0$.

(c) Prove by directly evaluating the variance matrices that although $Var(\underline{b}^0)$ generally depends on the choice of solution $\underline{b}^0$ that $Var(X\underline{b}^0)$ is the same for every solution. Under what condition does $Var(\underline{b}^0)$ not depend on the choice of the solution? $Var(\underline{b}^0) = Var(GX^T\underline{y}) = GX^TVar(\underline{y})(GX^T)^T = \sigma^2 GX^TXG^T$ which depends on G. $Var(X\underline{b}^0) = X\ Var(\underline{b}^0)X^T = \sigma^2$ $XG\ X^TXG^TX^T = \sigma^2 P_x(XG^TX^T)^T = \sigma^2 P_xP_x = \sigma^2 P_x$ is a function of X only, not on the solution. When X is full rank, the solution does not depend on G. G is unique.

(d) Use the result in (c) to conclude that $Var(\underline{q}'\underline{b}^0)$ is the same for every solution whenever $\underline{q}'$ is in the row space of X. $\underline{q}^T = \underline{s}^T X \Rightarrow Var(\underline{q}^T\underline{b}^0) = \underline{q}^T Var(\underline{b}^0)\underline{q} = \sigma^2 \underline{s}^T \overbrace{XGX^T}^{P_x}\overbrace{XG^TX^T}^{P_x}\underline{s} = \sigma^2\underline{s}^T P_x \underline{s}$ is not a function of G or $\underline{b}^0$.

4. (10 points) Do the following.

(a) Define what it means for a linear function $\underline{q}'\underline{b}$ to be estimable. $\underline{q}^T H = \underline{q}^T$. $\Re(\underline{q}^T) \subseteq \Re(X)$ i.e. $\underline{q}^T = \underline{s}^T X$.

(b) State two necessary and sufficient conditions for estimability. Use any one of them to probe that $\underline{q}'\underline{b}$ is estimable for every $\underline{q}$ in the full rank model. Further prove that if X does not have full rank, then there exists some $\underline{q}$ such that $\underline{q}'\underline{b}$ that is not estimable. i) X has full column rank. Therefore, $r(X) = p$. Therefore, every vector of length p is in $\Re(X)$. So, $\underline{q} \in \Re(X) \Rightarrow \underline{q}^T\underline{b}$ is estimable.

(c) Suppose that $\underline{q}_i'\underline{b}$ is estimable for $i = 1, 2, ..., r$. Let $a_1, a_2, ..., a_r$ be known constants. Can $\sum_{i=1}^r a_i\underline{q}_i'\underline{b}$ be non-estimable? If yes, give an example. If no, give a proof. No. $\underline{q}_i^T\underline{b}$ is estimable. Therefore, $\underline{q}_i^T H = \underline{q}_i^T \, \forall i \Rightarrow \underline{q}_i\underline{q}_i^T H = \underline{q}_i\underline{q}_i^T, \forall i \Rightarrow \sum \underline{q}_i\underline{q}_i^T H = \sum \underline{q}_i\underline{q}_i^T \Rightarrow \sum \underline{q}_i\underline{q}_i^T\underline{b}$ is estimable.

(d) Suppose that $\underline{q}_i'\underline{b}$ is non-estimable for $i = 1, 2, ..., r$. Let $a_1, a_2, ..., a_r$ by known constants. Can $\sum_{i=1}^r a_i\underline{q}_i'\underline{b}$ be estimable? If yes, give an example. If no, give a proof. One-way classification, for example. Yes.

5. (10 points) For the two-way nested classification model with $a = 3, b_1 = b_2 = b_3 = 2$, and arbitrary n_{ij},

(a) Find the quadratic form Q that appears in the numerator of the test statistic for testing H_0 : $\beta_{11} = \beta_{12}$.

(b) Specify the distribution of Q in (a), including its non-centrality. $\underline{b} = (\mu \;\; \alpha_1 \;\; \alpha_2 \;\; \alpha_3 \;\; \beta_{11} \;\; \beta_{12} \;\; \beta_{21} \;\; \beta_{22} \;\; \beta_{31} \;\; \beta_{32})^T$. $K^T = (0 \; 0 \; 0 \; 0 \; 1 \; -1 \; 0 \; 0 \; 0 \; 0)$. $H_0 : K^T\underline{b} = 0$. $K^T\underline{b}_0 = \underline{\bar{y}}_{11\cdot} - \bar{y}_{12\cdot\cdot}$ $K^TGK = \frac{1}{n_{11}} + \frac{1}{n_{12}}$.

$$Q = \frac{(\bar{y}_{11\cdot} - \bar{y}_{12\cdot})^2}{\frac{1}{n_{11}} + \frac{1}{n_{12}}} \sim \chi^{2\prime}\left(1, \frac{1}{2\sigma^2}\frac{(\beta_{11} - \beta_{12})^2}{(\frac{1}{n_{11}} + \frac{1}{n_{12}})}\right)$$

(c) Specify another hypothesis for which the Q is independent of that in (a), and prove independence. There are many choices. For example, take $K_2^T = (0 \; 0 \; 0 \; 0 \; 0 \; 0 \; 1 \; -1 \; 0 \; 0)$. K_1^T in part (a), then $K_1^T G K_2 = 0$.

15.24 Connectedness in 2-Way Crossed Classification

A 2-way crossed model with out interaction is said to be *connected* if the rank $r(X) = a + b - 1$. Recall that $r(X) \leq a + b - 1$.

Lemma 7.1: $\sum_{i=1}^a \ell_i\alpha_i$ is estimable. Therefore, $\sum_{i=1}^a \ell_i = 0$. Proof: $\sum_{i=1}^a \ell_i\alpha_i = \underline{\ell}^T\underline{\alpha}$ is estimable iff $\exists \underline{c} \ni$: $E(\underline{c}^T\underline{y}) = \underline{\ell}^T\underline{\alpha}$ iff $E(\underline{c}^T\underline{y}) = \underline{c}^T(\mu\underline{j}_{n\cdot\cdot} + A\underline{\alpha} + L\underline{\beta}) = \underline{\ell\alpha}$ iff $\underline{c}^T\underline{j}_{n\cdot\cdot} = 0$, $\underline{c}^T A = \underline{\ell}^T$, $\underline{c}^T L = 0 \Rightarrow \underline{\ell}^T\underline{j} = \underline{c}^T A\underline{j} = \underline{c}^T\underline{j}_{n\cdot\cdot} = 0$.

Lemma 7.2: If $\sum_{j=1}^b w_j\beta_j$ is estimable, then this implies $\sum_{j=1}^b w_j = 0$. The proof is similar to Lemma 7.1.

Lemma 7.3: $\underline{w}^T\underline{\beta}$ is estimable iff $\underline{w}^T \in \Re(F)$. Proof: From earlier, we know that the matrix H for absorbing the $\alpha's$ is

$$H_\alpha = \begin{pmatrix} 0 & \underline{0}_a^T & \underline{0}_b^T \\ \underline{j}_a & I_a & D(n_{i.}^{-1})N[I - \Im F] \\ \underline{0}_b & 0_{b\times a} & \Im F \end{pmatrix}.$$

Now, $\underline{q}^T\underline{b}$ is estimable iff $\underline{q}^T H_\alpha = \underline{q}^T$. Here, $\underline{q}^T = (0\ \underline{0}_q^T\ \ \underline{w}^T)$. So, $\underline{q}^T H_\alpha = (0\ \underline{0}_a^T\ \ \underline{w}^T \Im F) = (0\ \underline{0}_q^T\ \ \underline{w}^T)$ iff $\underline{w}^T = \underline{w}^T \Im F$ iff $\underline{w}^T \in \Re(F)$.

Lemma 7.4: $\underline{\ell\alpha}$ is estimable if $\underline{\ell}^T \in \Re(C)$ where $C = Diag(n_{i.}) - ND(n_{.j}^{-1})N^{-1}$. Proof: The proof is similar to Lemma 7.3, but use the H matrix which results from absorbing the $\beta' s$.

$$H_\beta = \begin{pmatrix} 0 & \underline{0}_a^T & \underline{0}_b^T \\ \underline{0}_a & \varrho C & 0 \\ \underline{j}_b & D(n_{.j}^{-1})N^T(I - \varrho C) & I_b \end{pmatrix}$$

Note that the Lemmas imply that $C\underline{j}_a = \underline{0}_a$ and $F\underline{j}_b = \underline{0}_b$.

Theorem 7.1: The following five statements are equivalent for a two-way crossed classification model without interaction.

1. The design is connected.
2. The rank $r(C) = a - 1$.
3. The rank $r(F) = b - 1$.
4. Every contrast of the $\alpha_i' s$ is estimable.
5. Every contrast of the $\beta_j' s$ is estimable.

Proof: $r(X) = r(X^T X) = r(H_\alpha) = a + r(\Im F) = a + r(F)$. Similarly, $r(X) = r(X^T X) = r(H_\beta) = b + r(\varrho C) = b + r(C)$. Hence, $r(X) = a+b-1 \Leftrightarrow r(F) \leq b-1 \Leftrightarrow r(C) = a-1$. Now, F is $b\times b$ and $F\underline{j}_b = \underline{0}_b \Rightarrow r(F) \leq b-1$. Lemma 7.3 says every contrast $\underline{w}^T\underline{\beta}$ is estimable $\Leftrightarrow r(F) = b-1$. Similarly, every contrast $\underline{\ell}^T\underline{\alpha}$ is estimable iff $r(C) = a - 1$. A *chain* for a two-way crossed classification is an alternating sequence of $\alpha' s$ and $\beta' s$ such that adjacent elements in the sequence occur together on at least one observation. So, $(\alpha_i\beta_j)$ is in the chain which implies that $n_{ij} \geq 1$.

Theorem 7.2: A two-way crossed classification model is connected iff every pair $(\alpha_i, \alpha_{i'})$ for $i \neq i'$ is connected by a chain iff every pair $(\beta_j, \beta_{j'})$ for $j \neq j'$ is connected by a chain. Proof: Suppose α_i and $\alpha_{i'}$ are in a chain. Create a corresponding chain of observations $y_{m1}, y_{m2}, ...$ so that y_{mt} receives the level of the α factor and of the β factor given by the t-th link in the chain.

	β_1	β_2	β_3	β_4
α_1	1	1		1
α_2		1	1	
α_3		1		1

Consider $\alpha_1\beta_2\alpha_3$ where $y_1 = \alpha_1\beta_2$ and $y_2 = \beta_2\alpha_3$. $(1,2),(2,3)$ is a chain. $E(y_1 - y_2) = (\mu + \alpha_1 + \beta_2) - (\mu + \alpha_3 + \beta_2) = \alpha_1 - \alpha_3$. Then, $E\left(\sum_t y_{mt}(-1)^{t+1}\right) = \alpha_i - \alpha_{i'}$. Suppose that some pair $(\alpha_i, \alpha_{i'})$ is not connected by a chain. Form equivalence classes on the $\alpha' s$ by $\alpha_i = \alpha_{i'}$ iff they are connected by a chain. By assumption, we get $d \geq 2$ equivalent classes $E_1, E_2, ..., E_d$ and $\alpha' s$ in different classes have no common $\beta's$ or else they would be connected by a chain. So, corresponding to the $E_t's$ there is also a partition of the $\beta's$ $D_1, D_2, ..., D_d$. Furthermore, we can partition the data $\underline{y}$ as $\underline{y}_1, \underline{y}_2, ..., \underline{y}_d$ where $E(\underline{y}_t)$ involves only $\alpha's$ and $\beta's$ in E_t and D_t. Let $\alpha_i \in E_1$ and $\alpha_{i'} \in E_2$. Suppose $\alpha_i - \alpha_{i'}$ is estimable. Then $\exists \underline{\ell}_1, \underline{\ell}_2 \ni$: $E(\underline{\ell}_1^T \underline{y}_1 + \underline{\ell}_2^T \underline{y}_2) = \alpha_i - \alpha_{i'} \Rightarrow E(\underline{\ell}_1^T \underline{y}_1) = \alpha_i$ and $E(\underline{\ell}_2^T \underline{y}_2) = \alpha_{i'}$ which contradicts Lemma 7.1.

Suppose we have a disconnected layout. Label the levels of the A factor so that

$$
\begin{aligned}
&\alpha_1, \alpha_2, ..., \alpha_{i1} \in E_1 \\
&\alpha_{i+1}, \alpha_{i+2}, ..., \alpha_{i2} \in E_2 \\
&\vdots \\
&\alpha_{id_1+1}, \alpha_{id_2+2}, ..., \alpha_{id} \in E_d
\end{aligned}
$$

Here, d is equal to the number of disconnected components. Label the $\beta_j's$ similarly. Then, the crossed classification will look like this.

	β_1 β_2 $\cdots$ β_{j_1}	β_{j_1+1} β_{j_1+2} $\cdots$ β_{j_2}	$\cdots$	β_{j_d+1} $\cdots$ β_{j_d}
α_1 α_2 α_{i1}	*connected*	*empty*	*empty*	*empty*
α_{i_1+1} α_{i_1+2} $\vdots$ α_{i_2}	*empty*	*connected*	*empty*	*empty*
$\vdots$	*empty*	*empty*	*connected*	*empty*
α_{d_1+1} α_{d_2+2} $\vdots$ α_d	*empty*	*empty*	*empty*	*connected*

There are d connected components, each of which is effectively a *separate* crossed classification, and which is analyzed separately (except for a pooled error term if desired). So hereto forth, we assume our layout is connected.

Estimable Functions

1. Any contrast $\sum_{i=1}^a \ell_i\alpha_i$ where $\sum_{i=1}^a \ell_i = 0$, $\sum_{i=1}^a \widehat{\ell_i\alpha_i} = \underline{\ell}^T \varrho(\underline{y}_a - N\underline{\bar{y}}_b)$, $Var(\sum_{i=1}^a \widehat{\ell_i\alpha_i}) = \underline{\ell}^T \varrho\underline{\ell}\sigma^2$.

2. Any contrast $\sum_{j=1}^b w_j\beta_j$ where $\sum_{j=1}^b w_j = 0$. Similar expressions for the B.L.U.E. and the variance exist.

3. $\mu + \alpha_i + \beta_j$ is estimable for $\forall i, j$.

So, a LIN set of $a + b - 1$ estimable functions is any $a - 1$ contrasts of $\alpha's$, any $b - 1$ contrasts of $\beta's$ and any single $\mu + \alpha_i + \beta_j$.

Hypothesis Testing

The hypotheses of interest are $H_0 : \beta_1 = \beta_2 = \cdots = \beta_b$ versus H_1 : not all equal. The null hypothesis may also be written as $H_0 : K^T\underline{b} = \underline{0}$ where $K^T = (\underline{0},\ 0_{(b-1)\times a},\ I_{b-1},\ -\underline{j}_{b-1})$. The null hypothesis $K^T\underline{b} = \underline{0}$ says $\beta_1 - \beta_b = 0$, $\beta_2 - \beta_b = 0, ..., \beta_{b-1} - \beta_b = 0$. We need $Q = (K^T\underline{b}^0)^T(K^TGK)^{-1}(K^T\underline{b}^0)$. $K^TG = (\underline{0}\ :\ (I_{b-1}, \underline{j}_{b-1})[-\Im N^T D(n_{i.}^{-1})]\ :\ (I_{b-1}, -\underline{j}_{b-1})\Im)$. But,

$$(I_{b-1},\ -\underline{j}_{b-1})\Im = (I_{b-1},\ -\underline{j}_{b-1})\begin{pmatrix} F_{b-1}^{-1} & \underline{0} \\ \underline{0} & 0 \end{pmatrix} = (F_{b-1}^{-1},\ \underline{0}) \Rightarrow$$

$$K^T G K = (\underline{0},\ (F_{b-1}^{-1}, 0)N^T D(n_{i.}^{-1})\ :\ (F_{b-1}^{-1}, \underline{0}))\begin{pmatrix} \underline{0}^T \\ 0 \\ I_{b-1} \\ -\underline{j}_{b-1}^T \end{pmatrix} = F_{b-1}^{-1} \Rightarrow$$

$$(K^T G K)^{-1} = F_{b-1} \Rightarrow Q = (K^T \underline{b}^0)^T F_{b-1} (K^T \underline{b}^0),$$

$$\underline{b}^{0^T} K = \underline{\beta}^{0^T}\begin{pmatrix} I_{b-1} \\ -\underline{j}_{b-1}^T \end{pmatrix} \Rightarrow Q = \underline{\beta}^{0^T}\begin{pmatrix} I_{b-1} \\ -\underline{j}_{b-1}^T \end{pmatrix} F_{b-1}(I_{b-1}, -\underline{j}_{b-1})\underline{\beta}^0,$$

$$\begin{pmatrix} I_{b-1} \\ -\underline{j}_{b-1}^T \end{pmatrix} F_{b-1}(I_{b-1}, -\underline{j}_{b-1}) = \begin{pmatrix} F_{b-1} & -F_{b-1}\underline{j}_{b-1} \\ -\underline{j}_{b-1}^T F_{b-1} & \underline{j}_{b-1}^T F_{b-1}\underline{j}_{b-1} \end{pmatrix} = F \text{ since } F \text{ has zero row and column sums } \Rightarrow$$

$Q = (\underline{y}_b - N^T \underline{\bar{y}}_a)^T \Im F \Im (\underline{y}_b - N^T \underline{\bar{y}}_a)$. You can check that for $\Im F \Im = \Im \Rightarrow Q = (\underline{y}_b - N^T \underline{\bar{y}}_a)^T \Im (\underline{y}_b - N^T \underline{\bar{y}}_a) = R(\beta|\mu, \alpha)$. Similarly, $R(\alpha|\mu, \beta)$ tests $H_0 : \alpha_1 = \alpha_2 = \cdots = \alpha_a$. What does $R(\alpha|\mu)$ test? $R(\alpha|\mu) = \sum_{i=1}^a n_{i.}\bar{y}_{i..}^2 - \frac{1}{n_{..}}\left(\sum_{i=1}^a y_{i..}\right)^2$. Recall $\underline{x}^T A \underline{x}$ has non-centrality $\frac{1}{2}(\mu^T A \mu)$ which implies that the non-centrality of

$$R(\alpha|\mu) = \sum_{i=1}^a n_{i.}\left(\mu + \alpha_i + \sum_{j=1}^b \frac{n_{ij}\beta_j}{n_{i.}}\right)^2 - \frac{1}{n_{..}}\left(n_{i.}\mu + \sum_{i=1}^a n_{i.}\alpha_i + \sum_{i=1}^a\sum_{j=1}^b n_{ij}\beta_j\right)^2.$$

Write

$$\theta_i = \mu + \alpha_i + \sum_{j=1}^b \frac{n_{ij}\beta_j}{n_{i.}}.$$

So, we have

$$\sum_{i=1}^a n_{i.}\theta_i^2 - \frac{1}{n_{..}}\left(\sum_{i=1}^a n_{i.}\theta_i\right)^2 =$$

$$\sum_{i=1}^a n_{i.}\left(\theta_i - \sum_{i=1}^a \frac{n_{i.}\theta_i}{n_{..}}\right)^2 =$$

$$\sum_{i=1}^a n_{i.}(\theta_i - \bar{\theta})^2$$

where $\bar{\theta} = \frac{\sum_{i=1}^a n_{i.}\theta_i}{n_{..}} = 0$ iff $\theta_1 = \theta_2 = \cdots = \theta_a$ iff $\alpha_i + \sum_{j=1}^b \frac{n_{ij}\beta_j}{n_{i.}}$ is equal for $i = 1, 2, ..., a$. That is the hypothesis tested by $R(\alpha|\mu)$ in the full model. If all of the $n_{ij}'s$ are equal, say to n, then $\theta_i = \mu + \alpha_i + \frac{n\sum_{j=1}^b \beta_j}{nb} = \mu + \alpha_i + \bar{\beta}_{..}$ So, $R(\alpha|\mu)$ tests $\alpha_1 = \alpha_2 = \cdots = \alpha_a$ when the data are balanced. Therefore, $R(\alpha|\mu, \beta) = R(\alpha|\mu)$ when $n_{ij} = n$. That's why only one ANOVA table is needed for balanced data.

15.25 Two-Way Crossed Classification with Interaction

The new model statement is $y_{ijk} = \mu + \alpha_i + \beta_j + \gamma_{ij} + \epsilon_{ijk}$. To compare this to the interaction model, write $\mu_{ij} = E(y_{ijk})$. Then, $\mu_{ij} - \mu_{ij'} = (\beta_j - \beta_{j'}) + (\gamma_{ij} - \gamma_{ij'})$ where $(\beta_j - \beta_{j'})$ does not depend on i and $(\gamma_{ij} - \gamma_{ij'})$ does depend on i. Thus, the differences of levels of B depend on the level A in the interaction model. But, they are the same for every level of A in the no-interaction model. Also, consider for another perspective the parameter

$$\theta_{ij,i'j'} = \mu_{ij} - \mu_{ij'} - \mu_{i'j} + \mu_{i'j'} = (\mu_{ij} - \mu_{ij'}) - (\mu_{i'j} - \mu_{i'j'}) =$$

$$\begin{cases} (\gamma_{ij} - \gamma_{ij'}) - (\gamma_{i'} - \gamma_{i'j'}), & \text{in the interaction model.} \\ 0, & \text{in the no intersection model.} \end{cases}$$

We will come back to the $\theta_{ij,i'j'}$'s. The test for interaction actually tests the $\theta_{ij,i'j'}$'s equal to zero.

Define the following.

$$\underline{\gamma}_{s\times 1} = \begin{pmatrix} \gamma_{11} \\ \gamma_{12} \\ \vdots \\ \gamma_{ab} \end{pmatrix}$$

where s is the number of non-empty cells. $\underline{y} = \mu\underline{j} + A\underline{\alpha} + L\underline{\beta} + M\underline{\gamma} + \underline{e}$ where M is $n_{\cdot\cdot} \times s$ given by

$$M_{\ell,r} = \begin{cases} 1, & \text{if } \ell\text{-th measurement in a cell corresponds to } r\text{-th } \delta_{ij} \text{ in } \underline{\delta}. \\ 0, & \text{otherwise.} \end{cases}$$

$$y = X\underline{b} + \underline{e}, \quad X = (\underline{j},\ A,\ L,\ M), \quad \underline{b} = \begin{pmatrix} \mu \\ \underline{\alpha} \\ \underline{\beta} \\ \underline{\delta} \end{pmatrix}$$

The rank $r(X) = r(M) = s$ is equal to the non-empty cells because $\underline{j}$ depends on A, L and A, L depends on M. $y_{ijk} = \mu_{ij} + e_{ijk}$. We say the design is *connected* if $r(\underline{j}_n, A, L) = a + b - 1$. This is the same definition as in the no-interaction model. We assume that we have a connected design. The normal equations are $X^TX\underline{b} = X^T\underline{y}$. Since all the rank is in matrix M, then let $X_1 = (\underline{j}, A, L)$,

$$X = (\underline{j}, A, L, M) = (X_1, M) \Rightarrow X^TX = \begin{pmatrix} X_1^TX_1 & X_1^TM \\ M^TX_1 & M^TM \end{pmatrix}.$$

We know that the rank $r(X) = r(X^TX) = s$.

$$M^TM = \begin{pmatrix} n_{11} & & & \\ & n_{12} & & \\ & & \ddots & \\ & & & n_{ab} \end{pmatrix} = D_{s\times s}(n_{ij})$$

Hence, a g-inverse of X^TX is

$$G = \left(\begin{array}{c|c} 0 & 0 \\ --- & --- \\ 0 & D^{-1}(n_{ij}) \end{array} \right), \quad X^T\underline{y} = \begin{pmatrix} X_1^T\underline{y} \\ --- \\ M^T\underline{y} \end{pmatrix} \Rightarrow \underline{b}^0 = GX^T\underline{y} = \begin{pmatrix} 0 \\ ------ \\ (M^TM)^{-1}M^T\underline{y} \end{pmatrix} =$$

$$\left.\begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ \bar{y}_{11\cdot} \\ \bar{y}_{12\cdot} \\ \vdots \\ \bar{y}_{ab\cdot} \end{pmatrix}\right\} \begin{matrix} 1+a+b \\ \\ \\ \\ \\ \\ s \end{matrix}$$

Sum of Squares for ANOVA

The only new term is $R(\delta|\mu,\alpha,\beta) = R(\mu,\alpha,\beta,\delta) - R(\mu,\alpha,\beta) = \sum_{i=1}^a \sum_{j=1}^b n_{ij}(\bar{y}_{ij\cdot})^2 - \sum_{i=1}^a n_{i\cdot} y_{i\cdot\cdot}^2 - (\underline{y}_a - N^T \underline{\bar{y}}_a)^T \Im(\underline{y}_b - N^T \underline{\bar{y}}_a)$ or as $\sum_{i=1}^a \sum_{j=1}^b n_{ij}(\bar{y}_{ij\cdot})^2 - \sum_{j=1}^b n_{\cdot j} y_{\cdot j\cdot}^2 - (\underline{y}_a - N\underline{\bar{y}}_b)^T \varrho (\underline{y}_a - N\underline{\bar{y}}_b)$.

Estimable Functions

These are the estimable functions assuming connectedness.

1. No function of just α_i's is estimable. Proof: $\underline{K}^T = (0, \underline{\ell}^T, \underline{0}_b^T, \underline{0}_s^T)$. $\underline{K}^T \underline{b} = \underline{\ell}^T \underline{\alpha}$. $\underline{K}^T H = K^T G(X^T X) = \underline{0}^T \neq \underline{K}^T$.

2. Similarly, no functions of just the β's are estimable.

3. $\mu_{ij} = \mu + \alpha_i + \beta_j + \delta_{ij}$ is the mean for cell (i,j) is estimable iff $n_{ij} > 0$. The B.L.U.E.'s are $\widehat{\mu}_{ij} = \bar{y}_{ij\cdot}$ and $Var(\widehat{\mu}_{ij}) = \frac{\sigma^2}{n_{ij}}$. The μ_{ij}'s are the basic estimable functions in the interaction model. There are $s = r(X)$ of them and they are LIN. So, every estimable function is a linear combination of the μ_{ij}'s.

4. $\sum_{j=1}^b k_{ij}\mu_{ij} = \mu + \alpha_i + \sum_{j=1}^b k_{ij}(\beta_j + \delta_{ij})$ where $\sum_{j=1}^b k_{ij} = 0$ and $k_{ij} = 0$ if $n_{ij} = 0$ is a general weighted mean of row i cell means. For example, take $k_{ij} = \frac{1}{m_i}$ where m_i is equal to the number of non-empty cells in row i. Therefore, $\mu + \alpha_i + \frac{1}{m_i}\sum_{j=1}^b (\beta_j + \delta_{ij})$, $n_{ij} \neq 0$. Another choice is $k_{ij} = \frac{n_{ij}}{n_{i\cdot}}$. Any of these may be thought of as defining *row effects* for a crossed classification model with interaction. The most natural definition of a row effect in the interaction model is $\sum_{j=1}^b \frac{\mu_{ij}}{b} = \mu + \alpha_i + \sum_{j=1}^b \frac{(\beta_j + \delta_{ij})}{b}$ iff every cell in the row i has data (i.e. non-empty). This demonstrates one of the difficulties caused by empty cells.

5. Similarly to (4), a general weighted mean of column j cell means is $\sum_{i=1}^a h_{ij}\mu_{ij} = \mu + \beta_j + \sum_{i=1}^a h_{ij}(\alpha_i + \delta_{ij})$ where $\sum_{i=1}^a h_{ij} = 0$ and $n_{ij} = 0 \Rightarrow h_{ij} = 0$. With the appropriate choice of h_{ij}'s, this defines a *column effect.*

6. If cells (i,j), (i,j'), (i',j), and (i',j') all have data, then we can estimate $\theta_{ij,i'j'} = \mu_{ij} - \mu_{i'j} - \mu_{ij'} + \mu_{i'j'} = \delta_{ij} - \delta_{i'j} - \delta_{ij'} + \delta_{i'j'}$. We will see that $R(\delta|\alpha,\beta,\mu)$ tests that the θ's equal 0.

7. $\phi_i = \sum_{j=1}^b \left[n_{ij}\mu_{ij} - \sum_{i'=1}^a \frac{n_{ij}n_{i'j}}{n_{\cdot j}} \mu_{i'j} \right]$. The ϕ_i's arise in the test corresponding to $R(\alpha|\mu,\beta)$. Write

$$\underline{\phi} = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_a \end{pmatrix} = (\underline{\alpha} + (A^T - ND(n_{\cdot j}^{-1})L^T)M\underline{\delta}$$

   In a connected design, there are exactly $a-1$ LIN ϕ_i's.

8. $\psi_j = \sum_{i=1}^a \left[n_{ij}\mu_{ij} - \sum_{j'=1}^b \frac{n_{ij}n_{ij'}}{n_{i\cdot}} \mu_{ij'} \right]$. The ψ_j's arise in the test corresponding to $R(\beta|\mu,\alpha)$. Write

$$\underline{\psi} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_b \end{pmatrix} = F\underline{\beta} + (L^T - ND(n_{i.}^{-1})A^T)M\underline{\delta}.$$

Hypotheses Tests

$H : \mu + \alpha_i + \sum_{j=1}^{b} \frac{n_{ij}(\beta_j+\delta_{ij})}{n_{i.}}$ is equal for $i = 1, 2, ..., a$. This is tested by $Q = R(\alpha|\mu)$. $H : \mu + \beta_j + \sum_{i=1}^{a} \frac{n_{ij}(\alpha_i+\delta_{ij})}{n_{.j}}$ is equal for $j = 1, 2, ..., b$. This is tested by $Q = R(\beta|\mu)$. $H : \phi_1 = \phi_2 = \cdots = \phi_a$ is tested by $Q = R(\alpha|\mu, \beta)$. $H : \psi_1 = \psi_2 = \cdots = \psi_b$ is tested by $Q = R(\beta|\mu, \alpha)$. H : any set of $s - a - b + 1$ LIN estimable functions of $\theta_{ij,i'j'}$'s all equal to 0 is tested with $Q = R(\delta|\mu, \alpha, \beta)$.

As in the no interaction case, we have two ANOVA tables as we fit $\underline{\alpha}$ before $\underline{\beta}$ (absorb the $\alpha's$) or fit $\underline{\beta}$ before $\underline{\alpha}$ (absorb the $\beta's$).

Source	d.f.	SS
Mean	1	$R(\mu) = \bar{y}_{...}^2$
$\alpha's$ given mean	$a-1$	$R(\underline{\alpha}\|\mu) = \sum_i n_{i.}\bar{y}_{i.}^2 - n_{..}(\bar{y}_{..})^2$
$\beta's$ given $\alpha's$ and mean	$b-1$	$R(\underline{\beta}\|\mu,\underline{\alpha}) = (\underline{y}_b - N^T\underline{\bar{y}}_a)^T \Im (\underline{y}_b - N^T\underline{\bar{y}}_a)$
$\gamma's$ given $\alpha's$ $\beta's$ mean	$s-a-b+1$	$R(\underline{\gamma}\|\mu,\underline{\alpha},\underline{\beta}) =$ see notes
Error	$n_{..} - s$	$SS(E) = \underline{y}^T\underline{y} - \sum_{i=1}^a \sum_{j=1}^b n_{ij}\bar{y}_{ij.}^2$
Total	$n_{..}$	$SS(T) = \sum_i \sum_j \sum_k y_{ijk}^2$

Source	d.f.	SS
Mean	1	$R(\mu) = \bar{y}_{...}^2$
$\beta's$ given mean	$b-1$	$R(\underline{\beta}\|\mu) = \sum_j n_{.j}\bar{y}_{.j.}^2 - n_{..}(\bar{y}_{...})^2$
$\alpha's$ given $\beta's$ and mean	$a-1$	$R(\underline{\alpha}\|\mu,\underline{\beta}) = (\underline{y}_a - N\underline{\bar{y}}_b)^T C (\underline{y}_a - N\underline{\bar{y}}_b)$
$\gamma's$ given $\beta's$ $\alpha's$ mean	$s-a-b+1$	$R(\underline{\gamma}\|\mu,\underline{\alpha},\underline{\beta}) =$ see notes
Error	$n_{..} - s$	$SS(E) = \sum_i \sum_j \sum_k y_{ijk}^2 - \sum_{i=1}^a \sum_{j=1}^b n_{ij}\bar{y}_{ij.}^2$
Total	$n_{..}$	$SS(T) = \sum_i \sum_j \sum_k y_{ijk}^2$

The hypotheses tested by $R(\underline{\alpha}|\mu, \underline{\beta})$ and $R(\underline{\beta}|\mu, \underline{\alpha})$ in a 2-way cross classification model layout with interaction do not have much appeal. When all the cells are filled, there are better tests to run. First notice when the $n_{ij}'s$ are all equal, the null hypothesis tested by $R(\underline{\alpha}|\mu, \underline{\beta})$ reduces to $H_0 : \alpha_i + \bar{\gamma}_{i.}$ equal for $i = 1, 2, ..., a$ which is an attractive hypothesis test; the problems arise when the $n_{ij}'s$ are not equal. In effect, the hypothesis tested by $R(\underline{\alpha}|\mu, \underline{\beta})$ changes depending on the sample sizes which is not usually desirable. However, so long as every $n_{ij} > 0$, the $\alpha_i + \bar{\gamma}_{i.}$ are all estimable. So we can test the H_0 shown above. We just need the right Q to do so. It is

$$Q = \sum_{i=1}^{a} \left\{ \frac{\left(\sum_{j=1}^{b} \bar{y}_{ij.}\right)^2}{\sum_{j=1}^{b} \frac{1}{n_{ij}}} \right\} - \frac{\left\{ \sum_{i=1}^{a} \left(\frac{\sum_{j=1}^{b} \bar{y}_{ij.}}{\sum_{j=1}^{b} \frac{1}{n_{ij}}} \right) \right\}^2}{\sum_{i=1}^{a} \frac{1}{\sum_{j=1}^{b} \frac{1}{n_{ij}}}}$$

Similarly, if all $n_{ij} > 0$ we can always test $H_0 : \beta_j + \bar{\gamma}_{.j}$ equal for all j. When the $n_{ij}'s$ are all equal, Q for this H_0 is $R(\underline{\beta}|\mu, \underline{\alpha})$. More generally, it is the expression symmetric to the Q displayed above (interchange the roles of i and j).

15.26 Homework

1. This problem refers to the two-way crossed classification model with no interaction.

   (a) Solve the normal equations by absorbing the $\beta's$ into the $\alpha's$ and using the constraint $\mu^0 = 0$. You should get the solution

$$\begin{pmatrix} 0 \\ C(\underline{y}_a - N\underline{\bar{y}}_b) \\ \underline{\bar{y}}_b - D(n_{\cdot j}^{-1})N'C(\underline{y}_a - N\underline{\bar{y}}_b) \end{pmatrix}$$

   where C is any generalized inverse of $C = D(n_{i\cdot}) - N(n_{\cdot j}^{-1})N'$. Starting with equation (2), $D(n_{\cdot j})\underline{\beta}^0 = \underline{y}_b - N^T\underline{\alpha}^0$. $\underline{\beta}^0 = D(n_{\cdot j}^{-1})[\underline{y}_b - N^T\underline{\alpha}^0]$. Going to equation (1), $D(n_{i\cdot})\underline{\alpha}^0 + ND(n_{\cdot j}^{-1})[\underline{y}_b - N^T\underline{\alpha}^0] = \underline{y}_a$. Then, $D(n_{i\cdot})\underline{\alpha}^0 + ND(n_{\cdot j}^{-1})\underline{y}_b - ND(n_{\cdot j}^{-1})N^T\underline{\alpha}^0 = \underline{y}_a$, $[D(n_{i\cdot}) - ND(n_{\cdot j}^{-1})N^T]\underline{\alpha}^0 = \underline{y}_a - ND(n_{\cdot j}^{-1})\underline{y}_b$. $C\underline{\alpha}^0 = \underline{y}_a - N\underline{\bar{y}}_b$. $\underline{\alpha}^0 = C[\underline{y}_a - N\underline{\bar{y}}_b]$. Put $\underline{\alpha}^0$ into equation (2). $N^TC[\underline{y}_a - N\underline{\bar{y}}_b] + D(n_{\cdot j})\underline{\beta}^0 = \underline{y}_b$, $D(n_{\cdot j})\underline{\beta}^0 = \underline{y}_b - N^TC[\underline{y}_a - N\underline{\bar{y}}_b]$, $\underline{\beta}^0 = D(n_{\cdot j}^{-1})[\underline{y}_b - N^TC[\underline{y}_a - N\underline{\bar{y}}_b]$. $\underline{\beta}^0 = \underline{\bar{y}}_b - D(n_{\cdot j}^{-1})N^TC[\underline{y}_a - N\underline{\bar{y}}_b]$.

   (b) Now show that for any $\underline{\ell} \in \Re(C)$, the variance of $\widehat{\underline{\ell}'\underline{\alpha}}$ is $\sigma^2\underline{\ell}'C\underline{\ell}$ which does not depend on the choice of C. HINT: First prove that $Var(\underline{y}_a - N\underline{\bar{y}}_b) = \sigma^2 C$.

   (c) State, but do not prove, the result corresponding to (b) for $Var(\widehat{\underline{w}'\underline{\beta}})$. $\sigma^2\underline{w}^T\Im\underline{w} = Var(\widehat{\underline{w}^T\underline{\beta}})$ for any $\underline{w}^T \in \Re(\Im)$.

   (d) Prove that $\widehat{\underline{\ell}_1'\underline{\alpha}}$ and $\widehat{\underline{\ell}_2'\underline{\alpha}}$ are independent if and only if $\underline{\ell}_1'C\underline{\ell}_2 = 0$.

   (e) Write down C for the case when all n_{ij} are equal. Show that the condition in (d) becomes $\underline{\ell}_1'\underline{\ell}_2 = 0$.

2. Show that the data in Table 7.1 on page 262 of the text book is connected. Do the same for the data in Table 7.6 on page 287 of the text book. Table 7.1 is as follow.

	β_1	β_2	β_3
α_1	18	12	24
α_2	–	–	9
α_3	3	–	15
α_4	6	3	18

The paths are as follow.

$\alpha_1, \beta_3, \alpha_2$
$\alpha_1, \beta_2, \alpha_4$
$\alpha_1, \beta_1, \alpha_3$
$\alpha_2, \beta_3, \alpha_3$
$\alpha_2, \beta_3, \alpha_4$
$\alpha_3, \beta_1, \alpha_4$

Thus, the $\alpha's$ are connected. By Theorem 7.2, the $\beta's$ are connected since the $\alpha's$ are connected. Table 7.6 is as follow.

	β_1	β_2	β_3	β_4
α_1	3	0	1	2
α_2	2	2	0	0
α_3	0	2	2	4

The paths are as follow.

$$\beta_1, \alpha_1, \beta_3$$
$$\beta_1, \alpha_2, \beta_2$$
$$\beta_1, \alpha_1, \beta_4$$
$$\beta_2, \alpha_3, \beta_3$$
$$\beta_2, \alpha_3, \beta_4$$
$$\beta_3, \alpha_1, \beta_4$$

The $\beta's$ are connected.

3. Do problem 10 on page 329 of the text book. Use SAS.

```
data winners;
input women $ men $ y;
cards;
p a 800
p c 900
p d 1000
q a 1300
r b 600
r c 1400
s a 1200
s b 1400
s c 1000
s d 2400
;

proc glm;
class women men;
model y = women men;
run;
```

```
                                          The SAS System         15:40 Saturday, August 30, 2008   1

                                         The GLM Procedure

                                      Class Level Information

                                  Class         Levels    Values

                                  women              4    p q r s

                                  men                4    a b c d


                              Number of Observations Read          10
                              Number of Observations Used          10

                                           The SAS System         15:40 Saturday, August 30, 2008   2

                                         The GLM Procedure

Dependent Variable: y

                                                Sum of
         Source                      DF         Squares     Mean Square    F Value    Pr > F

         Model                        6     1519090.909      253181.818       1.08    0.5152

         Error                        3      700909.091      233636.364

         Corrected Total              9     2220000.000


                          R-Square     Coeff Var      Root MSE        y Mean

                          0.684275      40.27995      483.3595      1200.000


         Source                      DF       Type I SS     Mean Square    F Value    Pr > F

         women                        3     720000.0000     240000.0000       1.03    0.4914 R(alpha | mu)
         men                          3     799090.9091     266363.6364       1.14    0.4584


         Source                      DF     Type III SS     Mean Square    F Value    Pr > F

         women                        3     879090.9091     293030.3030       1.25    0.4284 R(alpha | mu, beta)
         men                          3     799090.9091     266363.6364       1.14    0.4584
```

Chapter 16

Survival Analysis

Dr. Dahiya, Old Dominion University

Statistics 640, Fall 1997

Text used: Lee, Elisa T. (1992), *Statistical Methods for Survival Data Analysis, Second Edition,* John Wiley & Sons, Inc., New York, New York.

This chapter is under construction. Please be patient (RLG).

The office hours are on Monday and Wednesday from 2:00 to 3:00pm. Grading will be based on 3 homework sets worth 30%, a paper presentation and final project worth 15%, a midterm worth 20%, and a final exam worth 35%.

16.1 Censored Data

Analyzing data involves:

- Time to death.
- Relapse.
- Occurrence of disease.

Example: Let the random variable X be the time to develop cancer after asbestos exposure.

The random variable x has the pdf $f(x)$ usually. $x_1, x_2, ..., x_n$ is a random sample. Inferences are based on this random sample. We have n subjects on trial for occurrence of a disease. Since getting all n observations can take a long time, we censor the data. There are 3 types of censoring.

Figure 16.1: Type I censoring.

- Type I — Consider n animals in a test for a fixed time T. See Figure 16.1. Let y equal to the time to the event for a given animal. Let $f(y)\,dy$ be the density function of y. The random sample is $y_1, y_2, ..., y_n$ if we do not stop at time T. If there are r failures in the interval $(0, T)$, then $n-r$ observations are *censored observations.* The data becomes $x_1, x_2, ..., x_r, r$. What is the distribution of r? $r \sim binomial(n, p)$ where $p = P(y < T) = F(T)$. For a given $r, x_1, x_2, ..., x_r$, it is an ordered sample size of r from a distribution with the pdf $\frac{f(t)}{F(T)}$. The joint pdf of the sample is $g(x_1, x_2, ..., x_r, r) = P(r)\,P(x_1, x_2, ..., x_r|r) = \begin{pmatrix} n \\ r \end{pmatrix} F(T)^r[1-F(T)]^{n-r} r! \prod_{i=1}^r \frac{f(x_i)}{F(T)}$. Suppose that $y_1, y_2, ..., y_n$ is a random sample. The joint distribution is given by $\prod_{i=1}^n f(y_i)$. If $x_1 < x_2 < \cdots < x_n$ is an ordered sample, then the joint pdf is given by $n! \prod_{i=1}^n f(x_i), 0 < x_1 < x_2 < \cdots < x_n < \infty$. Look for the distribution of the order statistic which can be found in a text book on non-parametric statistics. The distribution of x_r which is th r^{th} order statistic is $cF(x_r)^{r-1} f(x_r)[1-F(x_r)]^{n-r}, 0 < x_r < \infty$ where the constant $c = \frac{n!}{(r-1)!(n-r)!}$. Then, $P(x_1, x_2, ..., x_r|r) = \frac{n!}{(n-r)!}[1-F(T)]^{n-r} \prod_{i=1}^r f(x_i), 0 < x_1 < x_2 < \cdots < x_r < T$. $F(y) = P(Y \le y)$. $1 - F(y) = s(y) = P(Y > y)$ is called the *survival function.*

- Type II — Suppose there are n animals in the test. For a fixed r, stop at the r^{th} failure. We want more than r animals in the test. The time the study takes is $E(x_r)$. It goes down as n increases. What is the joint pdf of $(x_1, x_2, ..., x_r)$? The joint pdf of $(x_1, x_2, ..., x_r)$ is $n! \prod_{i=1}^n f(x_i), 0 < x_1 < x_2 < \cdots < x_r < x_{r+1} < \cdots < x_n$. Then,

$$g(x_1, x_2, ..., x_r) = n! \prod_{i=1}^r f(x_i) \int_{x_r}^{\infty} \cdots \int_{x_{n-1}}^{\infty} \cdots \prod_{i=r+1}^n f(x_i) d_{x_{r+1}} \cdots d_{x_n} =$$

$$\frac{n!}{(n-r)!}[1-F(x_r)]^{n-r} \prod_{i=1}^r f(x_i), 0 < x_1 < x_2 < \cdots < x_r < \infty.$$

- Type III — The censored times are different times for different patients.

  - Case 1 — Assume fixed censoring times. Let the censoring times be $L_1, L_2, ..., L_n$. For the i^{th} instance either T_i or L_i will be observed. t_i equals the observation for the i^{th} person which equals $\min(T_i, L_i)$. Then, consider the observations $t_1, t_2, ..., t_n$. Define the function

$$\delta_i = \begin{cases} 1, & \text{if } T_i \le L_i \text{ (uncensored).} \\ 0, & \text{if } T_i > L_i \text{ (censored).} \end{cases}$$

Then our data pairs become $(t_i, \delta_i), i = 1, 2, ..., n$. What is the joint pdf? $f(y)$ is the density function of the time to death. $F(y) = P(Y \le y)$. $s(y) = P(Y > y) = 1 - F(y)$. The joint pdf of (t_i, δ_i) is $f(t_i)^{\delta_i} s(t_i)^{1-\delta_i}$. $P(t_i = L_i, \delta_i = 0) = P(\delta_i = 0) = P(T_i > L_i) = s(L_i)$. The joint pdf of $(t_1, \delta_1), (t_2, \delta_2), ..., (t_n, \delta_n)$ is

$$L = \prod_{i=1}^n f(t_i)^{\delta_i} s(t_i)^{1-\delta_i} = \prod_{i \in D} f(t_i) \prod_{i \in C} s(t_i)$$

by dividing $\{1, 2, ..., n\}$ into two sets $\{C, D\}$ called the *likelihood function.* C is the censored set. D is the death set. The data is $t_1, ..., t_r^+, t_{r+1}^+, t_{r+2}^+, ..., t_n^+$ where $+$ represents censored data. Then,

$$L = \prod_{i=1}^r f(t_i) \prod_{i=r+1}^n s(t_i^+).$$

Example: The sample is $3, 5, 6^+, 4, 4.5^+$. The 6^+ and 4.5^+ are censored times.

– Case 2 — Assume the censoring times are random. The censoring times are $L_1, L_2, ..., L_i, ..., L_n$. The death times are $T_1, T_2, ..., T_i, ..., T_n$. T_i is a random variable with the pdf $f(t)$ and the survival function $s(t) = 1 - F(t)$. L_i is a random variable with the pdf $g(t)$ and the survival function $G(t) = P(L > t)$. $t_i = \min(L_i, T_i)$. So, we have a bivariate sample $(t_i, \delta_i), i = 1, 2, ..., n$. The pdf of (t_i, δ_i) is

$$h(t_i, \delta_i) = \begin{cases} f(t_i)G(t_i), & \text{if } \delta_i = 1. \\ g(t_i)s(t_i), & \text{if } \delta_i = 0. \end{cases}$$

or $h(t_i, \delta_i) = [f(t_i)G(t_i)]^{\delta_i}[g(t_i)s(t_i)]^{1-\delta_i}$. Assume that T_i and L_i are independent for the pdf's to work. Then, $P(t_i = t, \delta_i = 1) = P(T_i = t, L_i > t) = P(T_i = t)P(L_i > t) = f(t_i)G(t)$. The likelihood function of the joint pdf of the sample used to estimate the parameters is

$$L = \prod_{i=1}^{n} h(t_i, \delta_i) = \prod_{i=1}^{n} [f(t_i)G(t_i)]^{\delta_i}[g(t_i)s(t_i)]^{1-\delta_i} =$$

Read the correction to the notes in this section on page 1108 to the likelihood function, also.

$$\overbrace{\prod_{i=1}^{n} f(t_i)^{\delta_i} s(t_i)^{1-\delta_i}}^{L_1} \overbrace{\prod_{i=1}^{n} g(t_i)^{1-\delta_i} G(t_i)^{\delta_i}}^{L_2}$$

We are not interested in the censoring distribution. Write the likelihood function as $L = L_1 \times L2$. We maximize L with respect to the parameters involved in $f(t)$. It is the same as maximizing L_1.

Example: Assume that $f(t) = \frac{1}{\theta}e^{-t/\theta}$. Then, $s(t) = e^{-t/\theta}$.

16.2 Survival Function

Let T be the random variable for the survival time. The distribution of T can be characterized by three different functions.

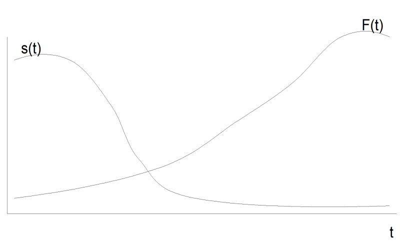

Figure 16.2: The survival function $s(t)$ versus $F(t)$.

1. The density function $f(t)\,dt$, $0 < t < \infty$.
2. The distribution function $F(t) = P(T \leq t) = \int_0^t f(x)\,dx$.
3. The survival function $s(t) = P(T > t) = 1 - F(t)$. This is the probability of dying after time t.

$$s(t) = \begin{cases} 1, & \text{if } t = 0. \\ 0, & \text{if } t = \infty. \end{cases}$$

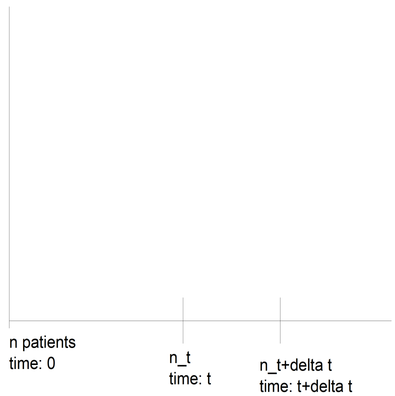

Figure 16.3: A non-parametric estimate of $s(t)$ based on n.

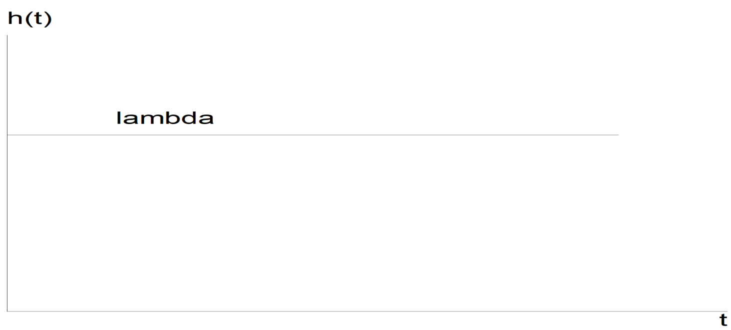

Figure 16.4: The hazard rate is constant because it has an exponential distribution.

See Figure 16.2.

How do we get a non-parametric estimate of $s(t)$ based on a sample of size n? See Figure 16.3. Let n_t equal to the number of patients surviving at time t. $\widehat{s}(t) = \frac{n_t}{n}$. How do we get the non-parametric estimate of $f(t)$?

$$f(t) = \lim_{\Delta t \to 0} \frac{P(T \in (t, t + \Delta t))}{\Delta t}$$

$$\widehat{f}(t) \frac{n_t - n_{t+\Delta t}}{n \Delta t}, t < t^* < t + \Delta t.$$

16.2.1 Hazard Function

The hazard function is the conditional failure rate.

$$h(t) = \frac{\lim P(T \in (t, t + \Delta t | T > t)}{\Delta t} = \lim_{\Delta t \to 0} \frac{P(T \in (t, t + \Delta t), T > t)}{P(T > t) \Delta t} =$$

$$\lim \frac{P(T \in (t, t + \Delta t))}{s(t)\Delta t} = \frac{f(t)}{s(t)} = \frac{f(t)}{1 - F(t)}.$$

This says, given a patient has survived to time t, what is the probability of dying in $(t, t + \Delta t)$?

Example: $T \sim exp(\lambda)$. Then, $f(t) = \lambda e^{-\lambda t}$. $F(t) = 1 - e^{-\lambda t}$. $s(t) = e^{-\lambda t}$. $h(t) = \frac{\lambda e^{-\lambda t}}{e^{-\lambda t}} = \lambda, \forall t > 0$. The hazard rate is constant iff T has an exponential distribution which means there is no aging or "old is as good as new." See Figure 16.4.

16.2.2 Estimation of $h(t)$ with Non-Parametric Methods

A non-parametric estimator of the hazard function is given by

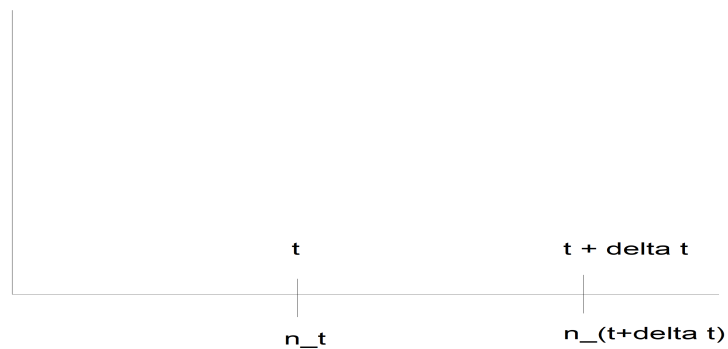

Figure 16.5: Non-parametric estimation of the hazard rate function.

$$\widehat{h}(t^*) = \frac{n_t - n_{t+\Delta t}}{n_t \Delta t} = \frac{\text{no. patients dying per unit of time in } (t, t + \Delta t)}{n_t} \text{ for } t < t^* < t + \Delta t.$$

An actuarial estimator of $h(t)$ is

$$\widehat{h}(t^*) = \frac{n_t - n_{t+\Delta t}}{\Delta t \left(n_t - \frac{(n_t - n_{t+\Delta t})}{2} \right)} = \frac{n_t - n_{t+\Delta t}}{\Delta t \frac{n_t + n_{t+\Delta t}}{2}}.$$

See Figure 16.5.

16.2.3 Cumulative Distribution Hazard Function

The cdf of the hazard function is given by

$$H(t) = \int_0^t h(x)\, dx = \int_0^t \frac{f(x)}{1 - F(x)}\, dx = \int_0^t -\frac{d}{dx} \log(1 - F(x))\, dx = -\log(1 - F(x))\Big|_0^t =$$

$$-\log(1 - F(x)) = -\log s(t) \Rightarrow e^{-H(t)} \Rightarrow f(t) = h(t)e^{-H(t)}.$$

See Figure 16.6.

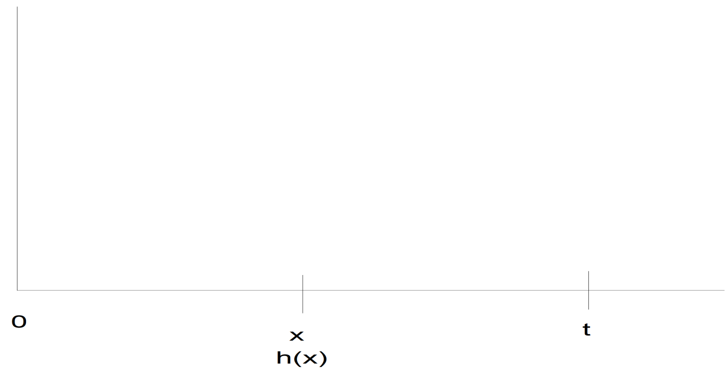

Figure 16.6: This figure shows the relationship between x and t.

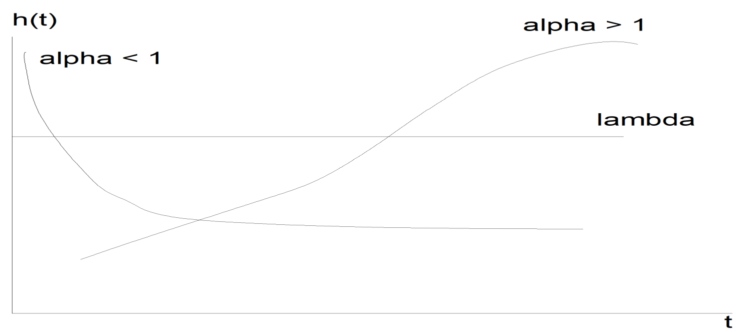

Figure 16.7: This figure shows the relationship between the exponential distribution and the Weibull distribution.

16.2.4 Behavior of $h(t)$ for Different Distributions

Here are some named distributions and their behavior as a hazard function. See Figure 16.7.

1. Exponential — $f(t) = \lambda e^{-\lambda t}$. $h(t) = \lambda$.
2. Weibull — $h(t) = \lambda\alpha(\lambda t)^{\alpha-1}, 0 < \alpha < \infty$ and $\lambda > 0$. For $0 < \alpha < 1, h(t)$ approaches infinity as t increases $h(t)$ decreases. For $\alpha > 1$, $h(t)$ increases as t increases. For $\alpha = 1$, $h(t) = \lambda$ which is the same as the exponential distribution. See Figure 16.8.

Example: This example appears on pages 13-15 in the text book. There are 40 myeloma patients. T is the survival time in months. The data is classified. See Figure 16.9.

t	total at risk	# died	$\widehat{f}(t), 0 < t < 5$
$(0, 5)$	40	5	$\frac{5}{40\times5} = 0.025$

$\widehat{h}^*(t) = \frac{5}{5\times\frac{40+35}{2}} = 0.027.$

16.3 Estimation of Survival Functions

$s(t) = P(T > t)$ assumes that all n patients have been observed. The ordered sample is $t_1 < t_2 < \cdots < t_n$. What is the non-parametric estimator for $s(t)$? Without making no assumption about the distribution of T

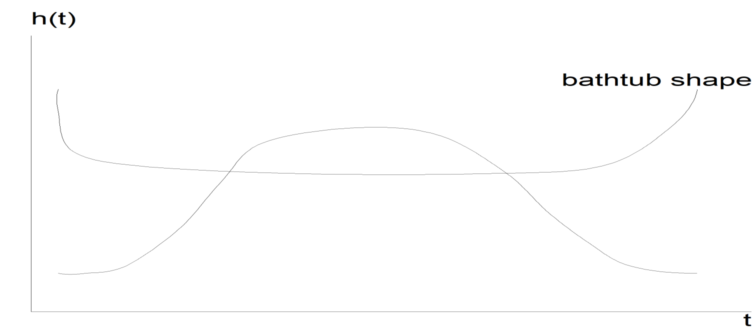

Figure 16.8: This figure shows the bathtub shape of the Weibull distribution.

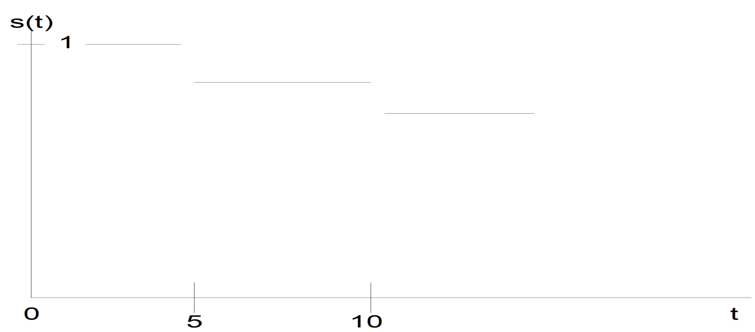

Figure 16.9: Text book example of 40 myeloma patients.

$\widehat{s}(t_i) = \frac{n-i}{n} = 1 - \frac{i}{n}$. If there are ties, then we use the largest i. $\widehat{s}(t_i) = \frac{\text{no. survived } t_i}{n}$.

Example: Let $t_5 = t_6 = t_7$. $\widehat{s}(t_5) = \frac{n-7}{n}$.

Some notes. $\widehat{s}(0) = 1, s(0) = 1, \widehat{s}(t_n) = 0$. and $\widehat{s}(t) = 1$ for $t < t_1$. See Figure 16.10 for plotting $\widehat{s}(t)$. $\tilde{s}(t)$ is using linear interpolation for $t_{i-1} < t < t_i$ used for estimating the median of T. $\tilde{s}(t)$ will be better. Suppose the data is classified. The *product limit estimator* is used. Assume n patients start at time zero and there is no censoring. The deaths are available in class intervals. No distribution is assumed for T. n_j is the number of patients at risk at time t_{j-1} which equals the number of patients surviving at time t_{j-1}. I_j equals the interval $[t_{j-1}, t_j) = \{t : t_{j-1} \le t < t_j\}$. d_j equals the number of deaths in I, $j = 1, 2, ..., k+1$. $t_{k+1} = \infty$, $t_0 = 0$. We have $k+1$ intervals. $p_j = P(T > t_j) = P(\text{patient survives } I_j) = s(t_j)$. $p_j = P(\text{survives } I_j | \text{survives } I_{j-1}) = \frac{p_j}{p_{j-1}}$. Let $q_j = 1 - p_j$. $p_j = p_j p_{j-1} \cdots = p_1 p_2 \cdots p_j$. Then, $s(t_j) = \prod_{i=1}^{j} p_i$. The sample data is $(d_1, d_2, ..., d_{k+1})$. To get the joint pdf, let $\pi_j = P(\text{death occuring in } I_j)$. Then, $\prod_{j=1}^{k+1} \pi_j = 1$. This has a multinomial distribution $(n, \pi_1, ..., \pi_{k+1})$. The likelihood function is

$$L = \frac{n!}{\prod_{j=1}^{k+1} d_j!} \prod_{i=1}^{k+1} \pi_j^{d_j}, \text{ where } \sum \pi_j = 1, \sum d_j = n.$$

$$\pi_j = P(t_{j-1} \le T < t_j) = F(t_j) - F(t_{j-1}) = 1 - s(t_j) - [1 - F(t_{j-1})] = s(t_{j-1}) - s(t_j) = p_{j-1} - p_j =$$

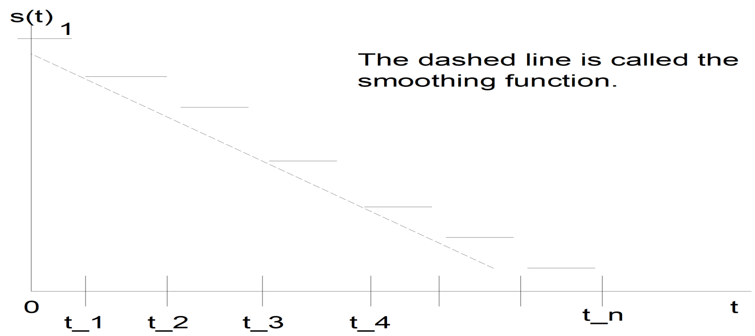

Figure 16.10: A smoothing function for $\tilde{s}(t)$.

$$\prod_{i=1}^{j-1} p_i - \prod_{i=1}^{j} p_i = p_1 p_2 \cdots p_{j-1}(1-p_j).$$

Let c be some constant. The likelihood function is

$$L = c\prod_{j=1}^{k+1}(p_1p_2\cdots p_{j-1}q_j)^{d_j} = c\prod_{j=1}^{k+1} q_j^{d_j} p_j^{n_j-d_j}.$$

The maximum estimate of p_j is $\sum_{j=1}^{k+1} p_j \neq 1$,

$$\frac{d\log L}{dp_j} = 0 \Rightarrow \widehat{p}_j = \frac{n_j-d_j}{n_j} \Rightarrow \widehat{q}_j = \frac{d_j}{n_j}.$$

$d_j|n_j \sum binomial(n_j, p_j)$. Then

$$\widehat{p}_j = \widehat{s}(t_j) = \prod_{i=1}^{j}\widehat{p}_i = \prod_{i=1}^{j}\frac{n_i-d_i}{n_i}.$$

Since $s(t_j) = P(T > t_j)$, then $\widehat{s}(t_j) = \frac{n_{j+1}}{n}$ where n_{j+1} equals the number of patients surviving to time t_j which equals $\frac{\pi_1-d_1}{n_1}\frac{n_2-d_2}{n_2}\cdots\frac{n_j-d_j}{n_j}$ where $n_i = n_{i-1}d_i$. Then after cancelations, $n_1 = n$ and $\frac{n_j-d_j}{n} = \frac{n_{j+1}}{n}$. $\widehat{p}_j = \frac{n_{j+1}}{n}$. $n_{j+1} \sim binomial(n, p_j)$. $E(\widehat{p}_j) = \frac{1}{n}E(n_{j+1}) = \frac{np_j}{n} = p_j$ and is unbiased. $Var(\widehat{p}_j) = \frac{p_j(1-p_j)}{n}$. $Cov(\widehat{p}_j, \widehat{p}_\ell) = \frac{(1-p_j)p_\ell}{n}, j < \ell$. The moments of $\widehat{q}_j$ are $\widehat{q}_j = \frac{d_j}{n_j}$, $d_j|n_j \sim binomial(n_j, q_j)$. d_j and n_j are random variables. Hypothetically, suppose that $E(yx) = E_x(xE(y|x))$. $E(y) = E_x[E(y|x)]$. Then, getting back to our problem, $E(\widehat{q}_j) = E\left(\frac{d_j}{n_j}\right) = E_{n_j}\left[\frac{1}{n_j}E(d_j|n_j\right] = E_{n_j}\left[\frac{1}{n_j}n_jq_j\right] = q_j$. Find $Var(\widehat{q}_j)$ using the property $Var(y) = E_x[Var(y|x)] + Var[E(y|x)]$. Then, $Var(\widehat{q}_j) = Var\left(\frac{d_j}{n_j}\right) = E_{n_j}\left[Var\left(\frac{k_j}{n_j}|n_j\right)\right] + Var\left[E\left(\frac{d_j}{n_j}|n_j\right)\right] = E_{n_j}\left[\frac{1}{n_j^2}Var(d_j|n_j)\right] + Var(q_j) = E_{n_j}\left[\frac{1}{n_j^2}n_jq_jp_j\right] + 0 = p_jq_jE\left(\frac{1}{n_j}\right)$. $n_j = 0$ is a possibility. If $n_j = 0$, then, $d_j = 0$ and $\frac{d_j}{n_j} = \frac{0}{0}$. Assume that $n_j > 0$. Let's consider the product limit estimator.

$$\prod_{i=1}^{j}\frac{n_i-d_i}{n_i}.$$

1. All n death times are available, $t_1 < t_2 < \cdots < t_n$ and $d_i = 1, i = 1, 2, ..., n$ because $k = n$. This implies $n_i = n - (i-1)$. Then, $\widehat{p} = \prod_{i=1}^{j} \frac{n_i - d_k}{n_i} = \prod_{i=1}^{j} \left(\frac{n_i - 1}{n_i}\right) = \prod_{i=1}^{j} \frac{n-(i-1)-1}{n-(i-1)} = \prod_{i=1}^{j} \frac{n-i}{n-i+1} = \frac{n-j}{n}$. We can write $\widehat{s}(t)$ for any t. $\widehat{s}(t) = \prod_{i:t_i \le t} \frac{n-i}{n-i+1}$. If j is the largest $t_i \le t$, then $\widehat{s}(t) = \frac{n-j}{n}$. Let n_i equal the number of dying patients upto time t. Then, $\widehat{s}(t) = \frac{n-n_{\tilde{t}}}{n}$. $\widehat{s}(t_j) = \prod_{i=1}^{j} \frac{n_i - d_i}{n_i} = \frac{n_{j+1}}{n}$.

16.4 Standard Life Estimators in Case of Withdraws or Censoring

Let w_j equal to the number of withdraws in I_j. $n_j = n_{j-1} - d_{j-1} - w_{j-1}$. Define $n'_j = n_j - \frac{w_j}{2}$ and $\widehat{p}_j = \frac{n'_j - d_j}{n'_j}$ and $\widehat{s}(t_j) = \prod_{i=1}^{j} \widehat{p}_i$.

Random Censoring and Likelihood Function

Let X equal to the life time and L equal to the censoring time. $f(x)$ is the pdf. $s(x) = P(X > x)$. $g(\ell)$ is the pdf. $G(\ell) = P(L > \ell)$. $T_i = \min(x_i, L_i)$. The data comes in as $(t_i, \delta_i), i = 1, 2, ..., n$. The likelihood function is

$$L = \prod_{i=1}^{n} f(t_i)^{\delta_i} s(t_i)^{1-\delta_i} \prod_{i=1}^{n} g(t_i)^{\delta_i} G(t_i)^{1-\delta_i},$$

$$L = c \prod_{i=1}^{n} f(t_i)^{\delta_i} s(t_i)^{1-\delta_i} = c \prod_{i=1}^{n} f(t_i)^{\delta_i} s(L_i)^{1-\delta_i}.$$

The Lee textbook uses $s(t) = P(T > t)$. The Lawless textbook uses $s(t) = P(T \ge t)$.

Product Limit Estimator of Kaplien and Mier

Let d_j equal to the deaths at time t_j. Let n_j equal to the number of individuals at risk $t_j - \epsilon$, for small $\epsilon > 0$. Let λ_j equal to the number of individuals censored in the interval $[t_{j-1}, t_j)$. L_i^j, $i = 1, 2, ..., j$ are the censoring times. Censoring at time t_j is considered to have occured just after time t_j. $F(t) = P(X \le t)$. $P(\text{death in } (t, t+dt)) = f(t)\,dt = F(t+dt) - F(t) = s(t) - s(t+dt)$.

$$L = c \prod_{i=1}^{n} f(t_i)^{\delta_i} s(L_i)^{1-\delta_i} = \prod_{i=1}^{k} [s(t_j - 0) - s(t_j)]^{d_j} \prod_{j=1}^{k+1} \prod_{i=1}^{\lambda_j} s(L_i^j), \quad \overbrace{\sum_{j=1}^{k} d_j}^{\text{deaths}} + \overbrace{\sum_{j=1}^{k+1} \lambda_j}^{\text{censors}} = n.$$

Non-Parametric Estimation

The number of parameters is $k + \sum_{i,j} \lambda_i^j$. We wish to maximize L with respect to the parameters

1. $\widehat{s}(t)$ where it must be discontinuous at death times t_i.
2. $\widehat{s}(t)$ where it must be as large as possible at censoring points.

$\widehat{s}(L_i^1) = 1,\ \ i = 1, 2, ..., \lambda_1$. $\widehat{s}(L_i^j) = \tilde{s}(t_{j-1}), i = 1, 2, ..., \lambda_j,\ \ j = 2, 3, ..., k+1$. Let $s(t_j) = p_j$. $s(t_j - \epsilon) = p_{j-1}$. Then, the likelihood function is

$$L = \sum_{j=1}^{k} (p_{j-1} - p_j) p_j^{\lambda_{j+1}}$$

because $\prod_{i=1}^{\lambda_j} s(L_i^j) = s(t_{j-1})^{\lambda_j}$ and

$$\prod_{j=1}^{k+1}\prod_{i=1}^{\lambda_j} s(L_i^j) = \prod_{j=1}^{k=1} s(t_{j-1})^{\lambda_j} = \prod_{j=2}^{k=1} s(t_{j-1})^{\lambda_j} = \prod_{i=1}^{k} s(t_i)^{\lambda_i}.$$

$$p_j = \frac{p_j}{p_{j-1}}.$$

Then,

$$L = c\prod_{j=1}^{k}(p_1p_2\cdots p_{j-1}q_j)^{d_j}(p_1p_2\cdots p_j)^{\lambda_{j+1}} = c\prod_{j=1}^{k} q_j^{d_j}p_j^{n_j-d_j},$$

$$\frac{d\log L}{dp_j} = 0 \Rightarrow \widehat{p}_j = \frac{n_j-d_j}{n_j}.$$

Note that $\lambda_j = n_{j-1} - n_j - d_{j-1}$ because $n_j = n_{j-1} - \lambda_j - d_{j-1}$. $s(t_j) = \prod_{i=1}^{j} p_i$. $\widehat{s}(t_j) = \prod_{i=1}^{j}\widehat{p}_i = \prod_{i=1}^{j}\left(\frac{n_i-d_i}{n_i}\right) = \frac{n_1-d_1}{n_1}\frac{n_2-d_2}{n_2}\cdots\frac{n_j-d_j}{n_j}$. Note that $n_2 = n_1 - d_1 - \lambda_1$ which implies that there is no cancelation here. For any t, $\widehat{s}(t) = \prod_{j:t_j\le t}\frac{n_j-d_j}{n_j}$. For any $t_{j-1} < t < t_j$, $\widehat{s}(t) = \prod_{i=1}^{j-1}\frac{n_i-d_i}{n_i}$.

Example: Given the trial times $t_1, t_2, t_3^+, t_4^+, t_5, t_6^+, t_7, t_8, t_9, t_{10}$, find the probability of survival.

i	$\widehat{s}(t_i)$
1	$\frac{9}{10}$
2	$\frac{9}{10}\frac{8}{9} = \frac{8}{10}$
3^+	$\frac{8}{10} = \widehat{s}(t_2)$
4^+	$\frac{8}{10} = \widehat{s}(t_2)$
5	$\widehat{s}(t_2)\frac{5}{6} = \frac{4}{6}$
6^+	$\widehat{s}(t_5) = \frac{4}{6}$
7	$\widehat{s}(t_5)\frac{3}{4} = \frac{1}{2}$
8	$\widehat{s}(t_7)\frac{2}{3} = \frac{1}{3}$
9	$\widehat{s}(t_8)\frac{1}{2} = \frac{1}{6}$
10^+	$\widehat{s}(t_9)$

Some notes.

1. $s(t)$ can not be estimated for $t > t_{10}^+$.
2. $s(t)$ can not be estimated for $t > L_{\lambda_{k+1}}^{k+1}$.

16.5 Properties of the Product Limit Estimator

The product limit estimator appears on pages 37-60 and page 75 of Lawless and in Chapter 4 of Lee.

Theorem: Let t be the upper limit on observation time and let censoring times and life times be independent and iid with continuous survivor functions $G(x)$ and $S(x)$. For $s(T) > 0$, the random function $\sqrt{n}[\widehat{s}(x) - s(x)] \to N(0, \sigma_s^2)$. For large n,

$$Var(\widehat{s}(x)) = \frac{\sigma_s^2}{n} = \frac{1}{n}s(x)^2 \int_0^x \frac{|d\, s(u)|}{s(u)s^0(u)},$$

where x equals to the lifetime, and L equals to the censoring time. $s^0(u) = P(X > u, L > u) = P(\text{individual at risk at time } u) = s(u)G(u)$. $\widehat{s}^0(u) = \frac{n_u}{n}$ is a binomial estimator.

16.5.1 Estimator of $Var(\widehat{s}(x))$

$$\widehat{Var}(\widehat{s}(x)) = \frac{1}{n}\widehat{s}(x)^2 \sum \frac{\widehat{s}(t_{j-1}) - \widehat{s}(t_j)}{\widehat{s}(t_j)\frac{n_j}{n}}$$

where n_j equals to the number of patients at risk at time t_j. $\widehat{s}(t_j) = \widehat{s}(t_{j-1})\frac{n_j - d_j}{n_j}$. Then,

$$\widehat{Var}(\widehat{s}(x)) = \frac{1}{n}\widehat{s}(x)^2 \sum_{j:t_j \le x} \frac{\widehat{s}(t_j)\frac{n_j}{n_j - d_j} - \widehat{s}(t_j)}{\widehat{s}(t_j)\frac{n_j}{n}} =$$

$$\widehat{s}(x)^2 \sum_{j:t_j \le x} \frac{d_j}{n_j(n_j - d_j)}.$$

Recall $h(t)\,dt = P(\text{dying in } (t, t+dt)|\text{ survives } t) = 0$ in between trial times. $\widehat{s}(t) = \prod_{j:t_j \le t} \frac{n_j - d_j}{n_j}$. The estimation of the Cumulative hazard function is $H(t) = -\log s(t)$. The mle is $\widehat{H}(t) = -\log \widehat{s}(t) = -\sum_{j:t_j \le t} \log\left(1 - \frac{d_j}{n_j}\right)$. $\tilde{h}(t_i) = \frac{d_i}{n_i}$. $\tilde{H}(t) = \sum_{j:t_j \le t} \frac{d_j}{n_j}$. We have two estimators for $H(t)$. For large n, $\widehat{H}(t) = \sum_{j:t_j \le t}\left(\frac{d_j}{n_j} + \frac{d_j^2}{2n_j^2} + \cdots\right)$ because $0 < x < 1$. $\log(1-x) = x + \frac{x^2}{2} + \frac{x^3}{3} + \cdots$. $\tilde{H} \approx \widehat{H}$ when ignoring $\Theta\left(\frac{1}{n_j^2}\right)$. $\tilde{h}(t_i)$ is called the *empirical hazard function.*

16.6 Life Tables

This section concerns the estimation of P_j when deaths and withdraws are classified. The interval I_j is defined as $I_j = [t_{j-1}, t_j), j = 1, 2, ..., k$ where there are k intervals. d_j equals to the number of deaths in I_j, w_j equals to the number of withdraws in I_j. n_j equals to the number of patients at risk at time t_{j-1} which is the same as the number of patients at risk during the interval I_j which is also equal to $n_{j-1} - d_{j-1} - w_{j-1}$. The probability $p_j = P(\text{patient survives past } I_j|\text{ survives } I_{j-1})$. $P_j = s(t_j) = P(\text{patient survives } I_j) = p_1 p_2 \cdots p_j$. For life table estimators, if there are no withdraws then $\widehat{q}_j = \frac{d_j}{n_j}$. In case of withdraws, all the $w_j's$ were not at risk during I_j. Assume $\frac{w_j}{2}$ were at risk during the interval I_j. $n'_j = n_j - \frac{w_j}{2}$ and $q'_j = \frac{d_j}{n'_j}$. Then, $\widehat{P}_j = \widehat{p}_1\widehat{p}_2 \cdots \widehat{p}_j = \frac{n'_j}{n'_j}$. $s(t)$ can not be estimated for $t_{j-1} < t < t_j$.

Theorem: Let $\theta' = (\theta_1, \theta_2, ..., \theta_k)$ be a parameter vector with estimator $\widehat{\theta}$. Let $\sqrt{n}(\widehat{\theta} - \theta) \to N(0, \Sigma)$. Let $g(\theta)$ be a function of $\theta_1, \theta_2, ..., \theta_k$ with the first derivate missing. Then, $\sqrt{n}(g(\widehat{\theta}) - g(\theta)) \to N(0, \sigma_g^2)$ where $\sigma_g^2 = \sum_i \sum_j \frac{dg}{d\theta_i}\frac{dg}{d\theta_j}\sigma_{ij}$ where $\Sigma = (\sigma_{ij})_{k \times k}$ is a $k \times k$ matrix. The asymptotic variance of $g(\theta)$ is $g(\widehat{\theta}) = \frac{1}{n}\sigma_g^2$. Use this theorem in the product limit estimator. $P_j = p_1 p_2 \cdots p_j$. $\widehat{p}_j = \frac{n_j - d_j}{n_j}$. $\widehat{P}_j = \widehat{p}_1\widehat{p}_2 \cdots \widehat{p}_j$. The distribution is $d_j|n_j \sim binomial(n_j, q_j)$. $\widehat{q}_j = \frac{d_j}{n_j}$. $E(\widehat{q}_j) = E_{n_j}\left[E(\widehat{q}_j|n_j)\right] = E_{n_j}\left[E\left(\frac{d_j}{n_j}|n_j\right)\right] = E_{n_j}\left[\frac{q_j n_j}{n_j}\right] = q_j \Rightarrow E(\widehat{p}_j) = 1 - E[\widehat{q}_j] = p_j$. $Var(\widehat{q}_j) = E_{n_j}\left[Var(\widehat{q}_j|n_j] + Var\left[E(\widehat{q}_j|n_j)\right]\right] = E_{n_j}\left[\frac{q_j p_j}{n_j}\right] + Var(q_j) =$

$q_j p_j E\left(\frac{1}{n_j}\right) + 0 \Rightarrow Var(\widehat{p}_j) = Var(\widehat{q}_j) = q_j p_j E\left(\frac{1}{n_j}\right) \Rightarrow Cov(\widehat{q}_j, \widehat{q}_i) = 0$. $\frac{\partial P_j}{\partial p_i} = p_1 p_2 \cdots p_{i-1} p_{i+1} \cdots p_j = \frac{P_j}{p_i} \Rightarrow Var(\widehat{P}_j) = \sum_{i=1}^{j} \left(\frac{d\,P_j}{d\,p_i}\right)^2 Var(\widehat{p}_i) = \sum_{i=1}^{j} \frac{P_j^2}{p_i^2} p_i q_i Var\left(\frac{1}{n_i}\right) = P_j^2 \sum_{i=1}^{j} \frac{q_i}{p_i} Var\left(\frac{1}{n_i}\right)$. The estimator for the variance $Var(\widehat{P}_j)$ is $\widehat{Var}(\widehat{P}_j) = \widehat{P}_j^2 \sum_{i=1}^{j} \frac{\widehat{q}_i}{\widehat{p}_i} \frac{1}{n_i} = \widehat{P}_j^2 \sum_{i=1}^{j} \frac{\frac{d_i}{n_i}}{1-\frac{d_i}{n_i}} \frac{1}{n_i} = \widehat{P}_j^2 \sum_{i=1}^{j} \frac{d_i}{n_i(n_i-d_i)}$. For the life tables, n_i is replaced by $n_i = n_i - \frac{w_i}{2}$.

16.6.1 Full Sample Case and the Product Limit Estimator

Suppose that $t_1 < t_2 < \cdots < t_n$. t_i^+ represents the i^{th} censored trial time. $\widehat{s}(t_j) = \widehat{p}_1 \widehat{p}_2 \cdots \widehat{p}_j$ where

$$\widehat{p}_i = \begin{cases} 1, & \text{if } i^{th} \text{ patient censored.} \\ \frac{n-i}{n-i+1}, & \text{if } i^{th} \text{ patient is a death.} \end{cases}$$

For any t, $\widehat{s}(t) = \prod_r \frac{n-r}{n-r+1}$ where r run through those positive integers where $t_r \leq t$ and t_r is uncensored. d_i equals 0 or 1. $\widehat{q}_i = \frac{1}{n-i+1}$.

Example: Let $n = 10$. The trial times and survival function are given next.

i	t_i	$\widehat{s}(t_i)$
1	t_1	$\frac{9}{10}$
2	t_2	$\frac{9}{10}\frac{8}{9}$
3	t_3^+	$\widehat{s}(t_2)$
4	t_4^+	$\widehat{s}(t_2)$
5	t_5	$\widehat{s}(t_2)\frac{5}{6}$
6	t_6^+	$\widehat{s}(t_5)$
7	t_7	$\widehat{s}(t_5)\frac{3}{4}$
8	t_8	$\widehat{s}(t_7)\frac{2}{3}$
9	t_9	$\widehat{s}(t_8)\frac{1}{2}$
10	t_{10}^+	$\widehat{s}(t_9)$

Example Consider the previous example and trial time 5. $\widehat{s}(t_5) = \frac{9}{10} \times \frac{8}{9} \times 56$. $\widehat{Var}(\widehat{s}(t)) = \widehat{s}(t)^2 \sum_{t_r \leq t} \frac{\widehat{q}_r}{\widehat{p}_r n_r} = \widehat{s}(t)^2 \sum_{r:t_r \leq t} \frac{1}{(n-r)(n-r+1)}$ which is the summation for uncensored trial times only.

Important Result: If the random variable X has a density function $f(x)$ with support on the real line $(0 < x < \infty)$, then

$$E(x) = \int_0^\infty x f(x)\,dx = \int_0^\infty (1 - F(x))\,dx = \int_0^\infty s(x)\,dx.$$

proof:

$$\int_0^T 1(F(T) - F(X))\,dx = |x(F(T) - F(x))|_0^T - \int_0^T -f(x) x\,dx = \int_0^T x f(x)\,dx, \;\; F(T) - F(x) \leq 1.$$

Taking the limit as $T \to \infty$, we have

$$\int_0^\infty 1 - F(x)\,dx = \int_0^\infty xf(x)\,dx.$$

Use the result in estimating $\mu = E(x)$ in censored data.

$$\mu = \int_0^\infty s(x)\,dx,$$

$$\widehat{\mu} = 1t_1 + (t_2 - t_1)\widehat{s}(t_1) + \cdots + (t_m - t_{m-1})\widehat{s}(t_{m-1}) + (t_n - t_m)\widehat{s}(t_m)$$

where t_m is the last death time and t_n^+ is the last censored time. For a random sample with no censoring, then $t_1, t_2, ..., t_n$, and $\widehat{\mu} = \bar{t}$, $Var(\widehat{\mu}) = \frac{\sigma^2}{n}$, and $\widehat{Var}(\widehat{\mu}) = \frac{\sum(t_i - \bar{t})^2}{n(n-1)}$. The Kaplan and Meier (1958) Journal of the American Statistical Association estimator is gives $\widehat{Var}(\widehat{\mu}) = \sum_{r=1}^m \frac{A_r^2}{(n-r)(n-r+1)}$ where A_r^2 equals to the area under the curve $\widehat{s}(t)$ to the right of t_r which equals $\sum_{k=r}^{m-1}(t_{k+1} - t_k)\widehat{s}(t_k) + (t_n - t_m)\widehat{s}(t_m)$. Some drawbacks of the Kaplan-Meier estimator include:

1. $\widehat{s}(t) = 0$ for $t \geq t_n$ if t_n is not censored. We know $s(t) > 0$.
2. The median estimator is an interval which is allowed. If $\widehat{s}(t) = 0.5$, $t_{i-1} \leq t < t_i$, then the interval $[t_{i-1}, t_i)$ is the estimator for the median. One can use linear interpolation to find the median.

16.6.2 Cohort Life Tables and Current Life Tables

A *cohort life table* involves a group of people born in the same year and following all of them to their death time. A *current life table* assumes that a person of age, say 20, will have the same chance of dying at age 50 as the current 50 year old. Notation: I_x equals the age interval $(x, x+t)$, where t is usually one year or 6 months. The probability of dying in interval q is ${}_tq_x = t_x^q =$ the death rate which equals to the proportion of age x people dying in the interval I_x. l_x equals to the number of people living at the beginning of the interval which equals $(1 -_t q_{x-t})l_{x-t}$. ${}_td_x$ equals the expected number of people dying in the interval I_x which equals $l_x({}_tq_x) = l_x - l_{x+t}$. We are assuming a stationary population. ${}_tL_x$ equals the number of person years the l_x persons live thru I_x which equals $t\left(l_{x+t} + \frac{1}{2t}dx\right)$. $T_x = \sum_{j \geq x} L_j$ equals the total number of years lived beyond age x by people alive at age x which equals ${}_tL_x + T_{x+t}$. e_x^0 equals the average remaining lifetime for the age x person which equals $\frac{T_x}{l_x}$. $x + e_x^0$ equals the expected age at death for the age x person. e_0^0 equals the life expectancy at birth.

Example: Consider the table on page 84 of the text book.

Column	
(1)	Age interval I_x, $t = 1$.
(2)	${}_tq_x$
(3)	l_x
(4)	${}_td_x$
(5)	${}_tL_x =_t L_{x+t} + \frac{1}{2}t\,dx$
(6)	Sum of (5) from bottom to top.
(7)	Column (6) divided by column (3) which equals $\frac{T_x}{l_x}$.

Expected Age at Death
$74.7 = x + l_x^0$
75.5
75.7
75.9 (15 - 20 interval)
$\vdots$
85.6 (75 - 80 interval)

x equals the age to death. Thus, the new column above is $E(X)$ is $E(X|X > x)$. It is the conditional life expectedness.

16.6.3 Clinical Life Tables

This section covers pages 87 thru 90 in the text book. l_i equals the number of people lost to follow-up in the i^{th} interval. w_i equals to the number of people withdrawn in the i^{th} interval. The following notation differs from the text book. $n_i = n_{i-1} - w_{i-1} - l_{i-1} - d_{i-1}$ equals to the number of people entering interval i. $n_i' = n_i - \frac{1}{2}(l_i + w_i)$ equals the effective number of people at risk during interval i. $b_i = t_i - t_{i-1}$ t_{m_i} equals to the mid-point of the i^{th} interval. $\widehat{s}(t_j) = \prod_{i=1}^{j} \widehat{p}_i$ is as it was before. $\widehat{q}_i = \frac{d_i}{n_i'}$.

1. $\widehat{f}(t_{m_i}) = \frac{\widehat{s}(t_{i-1}) - \widehat{s}(t_i)}{b_i} = \frac{\widehat{s}(t_{i-1})\widehat{q}_i}{b_i}$.
2. The hazard function estimator is is $h(t) = \frac{f(t)}{s(t)}$. $\widehat{h}(t_{m_i}) = \frac{\widehat{f}(t_{m_i})}{\widehat{s}(t_{m_i})} = \frac{1}{2}\left[\widehat{s}(t_{i-1}) - \widehat{s}(t_i)\right]$. The text book is using $\widehat{h}(t_{m_i}) = \frac{2\widehat{q}_i}{b_i(1+\widehat{p}_i)}$.

16.7 Relative and Corrected Survival Rates

The *relative survival rate* indexrelative survival rate equals to the observed survival rate for patients under study for a fixed period divided by the expected survival rate for the general population. Let $\widehat{p}$ be the survival rate for the i^{th} interval. n_i equals the number of people at risk during the i^{th} interval. p_{ij}^* equals the survival rate for the j^{th} individual in the control group of n_i people. $p_i^* = \frac{1}{n_i}\sum_{j=1}^{n_i} p_{ij}^*$. The relative survival rate equals $\frac{\widehat{p}_i}{p_i^*} > \widehat{p}_i$.

Example: See page 94 of the text book.

16.7.1 Corrected Survival Rates

Let p_c equal to the survival rate when cancer alone is the cause. p equals to the observed survival rate in patients under study. p_0 equals the survival rate for a control group. $p_c = \frac{p}{p_0}$. Consider two samples $x_{11}, x_{21}, ..., x_{n1}$ and $y_{12}, y_{22}, ..., y_{n2}$. x_i^+ will denote a censored observation. The tests of hypotheses are $H_0 : s_1(t) = s_2(t)$ versus $H_1 : s_1(t) > s_2(t)$ which implies treatment 1 is better or $H_1 : s_2(t) > s_1(t)$ which implies treatment 2 is better. The non-parametric test of Gehan's generalized Wilcoxon test for censored data is as follow. Look at the pairs (x_i, y_j), $i = 1, 2, ..., n_1$, $j = 1, 2, ..., n_2$.

$$u_{ij} = \begin{cases} 1, & \text{if } x_i > y_j \text{ or } x_i^+ \geq y_j. \\ -1, & \text{if } x_i < y_j \text{ or } x_i \leq y_j^+. \\ 0, & \text{otherwise.} \end{cases}$$

$E(y_{ij} = 0$ if H_0 is true. $E(u_{ij}|H_0) = 0$. $w = \sum_j \sum_i u_{ij}$. Consider the Mantel test (1967). Combine all $n_1 + n_2$ observations and order them. Define u_i equal to the number of observations i^{th} definitely greater than minus the number of observations i^{th} definitely less-than, $i = 1, 2, ..., n_1 + n_2$. Let $u_1, u_2, ..., u_{n_1}$ be the scores for the $x_i's$ Then, $w = \sum_{i=1}^{n_1} u_i$. All $\left(\begin{array}{c} n_1 + n_2 \\ n_1 \end{array}\right)$ possible arrangements have the chance. Under H_0,

$$\widehat{\sigma}_w^2 = \frac{n_1 n_2 \sum_{i=1}^{n_1+n_2} w_i^2}{(n_1+n_2)(n_1+n_2-1)}.$$

$E(w|H_0) = 0$. $\frac{w}{\widehat{\sigma}_w} \to N(0, 1)$.

Example: The sample sizes are $n_1 = 3$, $n_2 = 4$. The ordered sample is $2.0, \underline{2.5}, 3.5^+, \underline{4.0}, \underline{4.3^+}, 5.0, 6.0^+$.

trial	u_i
2.0	−6
2.5	−4
3.5^+	2
4.0	−1
4.3^+	3
5.0	2
6.0^+	4

$w = -4 - 1 + 3 = -2$. $\hat{\sigma}_w^2 = \frac{3\times4\times(36+16+4+1+9+4+16)}{6\times7} = 24.57$. $z = \frac{w}{\hat{\sigma}_w} = \frac{-2}{\sqrt{24.57}} = -0.40$. $H_1 : s_1 < s_2$. Reject H_0 at $\alpha = 0.05$ if $z < -1.64 \Rightarrow$ accept H_0. There is no difference.

16.7.2 Cox-Mantel Test

This section covers the Cox-Mantel test for $H_0 : s_1 = s_2$ Cox (1972), Journal of Royal Stat Society, Serv B, 34, p 187-202, "Distribution Free Methods for Proportional Hazards and Related Regression Models." Lawless Chapter 7 gives a summary. Let T equal the survival time. Besides the treatment, T is affected by other covariates of the individual patient. Let $X = (x_1, x_2, ..., x_p)$ be a vector of p covariates. The covariates are associated with the risk of the individual. The proportional hazard model assumes $h(t|x) = h_0(t)\exp(x, \beta)$ where $\beta^T = (\beta_1, \beta_2, ..., \beta_b)$ is a vector of parameters. $h_0(t)$ is the base hazard function. $h(t|x = 0) = h_0(t)$. The *baseline survival function* is

$$s_0(t) = \exp\left\{-\int_0^t h_0(u)\,du\right\} = e^{-H_0(t)}$$

The individual survival function is

$$s(t|x) = \exp\left\{-\int h_0(u)\exp(x\beta)\,du\right\} = [s_0(t)]^{\exp(x\beta)}.$$

How do we estimate the parameters $(\beta_1, \beta_2, ..., \beta_p)$? Let n subjects yield a sample of k distinct deaths and $n - k$ censored observations. Let R_i equal to the risk at time t_i. Cox suggested to use the *conditional* likelihood function. Let $x_{(i)}$ equal to the observation on the person dying at time t_i. Then,

$$\frac{e^{x_{(i)}\beta}}{\sum_{\ell\in R_i} e^{x_\ell \beta}} = P(\text{that particular person dies at } t_i).$$

The likelihood function of β is

$$\prod_{i=1}^{k} \frac{e^{x_{(i)}\beta}}{\sum_{\ell\in R_i} e^{x_\ell \beta}} = L(\beta).$$

This is the conditional likelihood given the death times $t_1, t_2, ..., t_k$. Estimators of β are functions of the covariates and R_i. $\frac{d\log L}{d\beta_j} = 0, j = 1, 2, ..., p$ gives p equations.

$$\log L = \sum_{i=1}^{k} x_{(i)}\beta - \sum_{i=1}^{k} \log \sum_{\ell\in R_i} e^{x_{(\ell)}\beta},$$

$$\frac{d\log L}{d\,\beta_j} = x_{ij} - \sum_{i=1}^{k} \frac{1}{\sum_{\ell\in R_i} e^{x_{(\ell)}\beta}} \left(\frac{d}{d\,\beta_j} \sum_{\ell\in R_i} e^{x_{(\ell)}\beta} \right)$$

The expression in the parentheses is the estimate of p non-linear equations to solve for $\beta_1, \beta_2, ..., \beta_p$. Let $\widehat{\beta}$ be the mle of β and for large n, let $\not\Sigma_{\widehat{\beta}}$ be the covariate matrix of $\widehat{\beta}$. From the theory of maximum liklihood gives

$$\not\Sigma_{\widehat{\beta}} = \left(\frac{-d^2 \log L}{d\,\beta_j\, d\beta_i} \right)_{\beta=\widehat{\beta}}$$

16.7.3 Cox Proportional Hazards Model

The new class time will be 10:15 to 11:30am.

The Cox proportional hazards model is used in testing the hypothesis $H_0 : s_1 = s_2$. x and β are scalars. $s(t) = [s_0(t)]^{e^{x\beta}}, x = 0$ or $x = 1$. For $x = 0$, we get $s(t) = s_0(t) = s_1(t)$. For $x = 1$, we get $s(t) = [s_0(t)]^{e^{\beta}}] = s_2(t)$. $H_0 : s_1(t) = s_2(t)$ is the same as $H_0 : \beta = 0$. Here are some special cases of the Cox proportional hazard model. Recall that the likelihood function is

$$L(\beta) = \prod_{i=1}^{k} \frac{e^{x_{(i)}\beta}}{\sum_{\ell\in R_i} e^{x_\ell \beta}}.$$

The data comes in at multiple deaths d_i at time t_i :

$$\begin{array}{cccc} t_1 & t_2 & \cdots & t_k \\ d_1 & d_2 & \cdots & d_k \end{array}$$

$\sum_{i=1}^{k} d_i = n$. Then,

$$L(\beta) = \prod_{i=1}^{k} \prod_{j=1}^{d_i} \left[\frac{e^{x_{(ij)}\beta}}{\sum_{\ell\in R_i} e^{x_{x_{(\ell)}}\beta}} \right]$$

Let $\sum_{j=1}^{d_i} x_{(ij)} = s_i$. Then,

$$L(\beta) = \prod_{i=1}^{k} \frac{e^{s_i \beta}}{\left[\sum_{\ell\in R_i} e^{x_{x_{(\ell)}}\beta}\right]^{d_i}} \frac{d\log L}{d\,\beta_j}, j = 1, 2, ..., p.$$

Another special case involves two populations. $s_2(t) = [s_1(t)]^{e^{\beta}}$.

times	t_1	t_2	$\cdots$	t_k
deaths	d_1	d_2	$\cdots$	d_k
at risk	n_1	n_2	$\cdots$	n_k

$d_i = \overbrace{d_{1i} + d_{2i}}^{\text{2 populations}}$. $n_i = n_{1i} + n_{2i}$. Then, the likelihood function $L = \prod_{j=1}^{d_i} e^{x_{(ij)}\beta}$ can be simplified. Note that $\sum_{j=1}^{d_i} x_{(ij)} = \sum_{j=1}^{d_{1i}+d_{2i}} x_{(ij)} = d_{2i}$, $\sum_{\ell=1}^{n_i} e^{x_{(\ell)}\beta}, x_{(\ell)} \in \{0,1\} = \sum_{\ell=1}^{n_{1i}+n_{2i}} e^{x_{(\ell)}\beta} = n_{1i} + n_{2i}e^{\beta}$. Now,

$$L = \prod_{i=1}^{k} \frac{e^{d_{2i}\beta}}{(n_{i1} + n_{2i}e^{\beta})^{d_i}},$$

$$\log L = \sum_{i=1}^{k} d_{2i}\beta - \sum_{i=1}^{k} d_i \log(n_{1i}(n_{1i} + n_{2i}e^{\beta}),$$

$$\frac{d\,\log L}{d\,\beta} = \sum_{i=1}^{k} d_{2i} - \frac{\sum_{i=1}^{k} d_i n_{2i} e^{\beta}}{n_{1i} + n_{2i}e^{\beta}}$$

$$\frac{-d^2\,\log L}{d\,\beta^2} = \frac{\sum_{i=1}^{k} d_i n_{2i} n_{1i} e^{\beta}}{(n_{1i} + n_{2i}e^{\beta}} = I(\beta).$$

The hypothesis being tested is $H_0 : \beta = 0$.

$$\frac{\frac{d\,\log L}{d\,\beta}}{\sqrt{I(\beta)}} \to N(0,1) \text{ as } n \to \infty.$$

$U(\beta) = \frac{d\,\log L}{d\,\beta}$. Under H_0, $z = \frac{u(0)}{\sqrt{I(0)}}$. This is the Cox-Mantel test for $H_0 : s_1(t) = s_2(t)$. See Lee page 108. To continue on,

$$u(0) = \sum_{i=1}^{k} d_{2i} - \frac{\sum_{i=1}^{k} d_i n_{2i}}{n_{1i} + n_{2i}} = r_2 - \sum_{i=1}^{k} \frac{d_i n_{2i}}{n_{1i} + n_{2i}}$$

$$I(0) = \frac{\sum_{i=1}^{k} d_i n_{1i} n_{2i}}{n_i^2}.$$

If there are too many ties, then a modified $I(0)$ is

$$I(0) = \sum_{i=1}^{k} \frac{d_i(n_i - d_i)n_{1i}n_{2i}}{n_i^2(n_i - 1)}$$

is modified for ties or test with $\sqrt{I(0)}(\widehat{\beta} - 0) \to N(0,1)$ under H_0. But you need to solve for $\widehat{\beta}$, again. Doing algebra $u(0)$, we obtain

$$u(0) = \sum_{i=1}^{k} \left(d_{2i} - \overbrace{\frac{d_i n_{2i}}{n_i}}^{\text{con'd mean}} \right)$$

Given n_i and given d_i under H_0,

$$E\left(d_{2i} | n_i, d_i, H_0\right) = \frac{d_i n_{2i}}{n_i} \Rightarrow u(0) = \sum_{i=1}^{k} (d_{2i} - E(d_{2i} | n_i d_i)).$$

16.7.4 m-Sample Test

We wish to test $H_0 : s_1(t) = s_2(t) = \cdots = s_m(t)$. Again, us the proportional hazard model. $s(t|x) = [s_0(t)]^{e^{x\beta}}$, $x = (x_1, x_2, ..., x_m)$ which are m vectors $(1, 0, ..., 0)$, $(0, 1, ..., 0)$, $(0, 0, ..., 1)$. Then, $s_m(t) = s_0(t)$, $s_1(t) = [s_0(t)]^{e^{\beta_1}} = [s_0(t)]^{\lambda_1}$; $\lambda_j = e^{\beta_j}$, $s_j(t) = [s_0(t)]^{\lambda_j}$, $j = 1, 2, ..., m-1$. The null hypothesis can be written in two ways $H_0 : \beta_1 = \beta_2 = \cdots = \beta_{m-1} = 0$ or as $H_0 : \lambda_1 = \lambda_2 = \cdots = \lambda_{m-1} = 1$. The data is

times	t_1	t_2	$\cdots$	t_k
deaths	d_1	d_2	$\cdots$	d_k
at risk	n_1	n_2	$\cdots$	n_k

$d_i = \sum_{j=1}^{m} d_{ji}$ and $n_i = \sum_{j=1}^{m} n_{ji}$. The likelihood function is

$$L(\beta) = \prod_{i=1}^{k} \prod_{j=1}^{d_i} \frac{e^{x_{(ij)}\beta}}{\sum_{\ell \in R_i} e^{x_{(\ell)}\beta}}.$$

What is $\sum_{j=1}^{d_i} x_{(ij)}\beta = d_{1i}\beta_1 + d_{2i}\beta_2 + \cdots + d_{m-1i}\beta_{m-1}$? What is $\sum_{\ell \in R_i} e^{x_{(\ell)}\beta} = n_{mi} + \sum_{j=1}^{m-1} n_{ji}e^{\beta_j}$? Then,

$$L(\beta) = \prod_{i=1}^{k} \frac{e^{\sum_{j=1}^{m-1} d_{ji}\beta_j}}{\left[n_{mi} + \sum_{j=1}^{m-1} n_{ji}e^{\beta_j}\right]^{d_i}}$$

$$\log L = \sum_{i=1}^{k} \sum_{j=1}^{m-1} d_{ji}\beta_j - \sum_{i=1}^{k} d_i \left(n_{mi} + \sum_{j=1}^{m-1} n_{ji}e^{\beta_j} \right).$$

Let $\sum_{i=1}^{k} d_{ji} = r_j$ equal to the total deaths from the j^{th} sample.

$$\frac{d\log L}{d\beta_j} = r_j - \frac{\sum_{i=1}^{k} d_i n_{ji} e^{\beta_j}}{n_{mi} + \sum_{i=1}^{k} n_{ji}e^{\beta_j}}.$$

Under $H_0 : \beta = 0$,

$$u_j(0) = \left.\frac{d\log L}{d\beta_j}\right|_{\beta=0} = r_j - \sum_{i=1}^{k} \frac{d_i n_{ij}}{n_i} = \sum_{i=1}^{k} \left(d_{ji} - \frac{d_j n_{ji}}{n_i} \right).$$

Also,

$$I_{j\ell}(0) = -\left.\frac{d^2\log L}{d\beta_j d\beta_\ell}\right|_{\beta=0} = \sum_{i=1}^{k} d_i \frac{n_{ji}}{n_i} \left(\delta_{j\ell} - \frac{n_{\ell i}}{n_i} \right)$$

where

$$\delta_{j\ell} = \begin{cases} 1, & \text{if } j = \ell \\ 0, & \text{otherwise} \end{cases} \quad \text{under } H_0.$$

$u(0)I^{-1}(0)u^T(0) \to \chi^2(m-1)$ where $u(0) = [u_1(0), ..., u_{m-1}(0)]$, $I(0) = (I_{j\ell}(0))_{(m-1)\times(m-1)}$.

16.7.5 Estimation of $s(t|x)$ for the Cox Proportional Hazard Model

Homework 1 is due on October 6. Homework 2 is due on October 15. The midterm exam will be on October 22.

The section references on Lawless, page 360. We have seen how to estimate β.

$$L=\prod_{j=1}^{k}\prod_{i=1}^{\lambda_j}[s(L_i^j)][s(t_j-0)-s(t_j)]^{d_j}\prod_{i=1}^{\lambda_{k+1}}s(L_i^{k+1}).$$

Now $s(t|x)=[s_0(t)]^{e^{x\beta}}$. x corresponds to the individual. Therefore, the expression represents different survival functions.

$$L=\left\{\prod_{j=1}^{k}\prod_{i=1}^{\lambda_j}[s(L_i^j|x_{(i)}^j)]\prod_{\ell\in D_j}[s(t_k-0|x_{(\ell)})-s(t_j|x_\ell)]\right\}\prod_{i=1}^{\lambda_{k+1}}s(L_i^{k+1}|x_{(i)}^{k+1}),$$

where D_j is the set of individuals dying at time t_j. $\widehat{s}_0(L_i^1)=1$, $i=1,2,...,\lambda_1$ and in general, $\widehat{s}_0(L_i^{j+1})=\widehat{s}_0(t_j)$, $j=1,2,...,k$; $i=1,2,...,\lambda_{j+1}$. Write $s_0(t_j)=P_j$. Then, $s_0(t_j|x)=P_j^{e^{x\beta}}$. Then, the likelihood function becomes

$$L=\prod_{j=1}^{k}\prod_{\ell\in C_j}P_{j-1}^{\exp\left\{x_{(\ell)}\beta\right\}}\prod_{\ell\in D_j}\left\{P_{j-1}^{e^{x_\ell\beta}}-p_j^{e^{x_\ell\beta}}\right\}\prod_{\ell=1}^{\lambda_{k+1}}P_k^{\exp\{x_\ell\beta\}}$$

where c_j equals to the set of individuals with censoring times in the interval $(t_{j-1},t_j]$, D_j equals to the set of individuals with death times in the interval $(t_{j-1},t_j]$. Let $\alpha_j=\frac{P_j}{P_{j-1}}$ where $P_{j-1}=\alpha_1\alpha_2\cdots\alpha_{j-1}$. Then, the likelihood function becomes

$$L=\prod_{j=1}^{k}\prod_{\ell\in C_j}(\alpha_1\alpha_2\cdots\alpha_{j-1})^{e^{x_\ell\beta}}\prod_{\ell\in D_j}\left(P_{j-1}^{e^{x_\ell\beta}}-\alpha_jP_{j-1}^{e^{x_\ell\beta}}\right)\prod_{\ell=1}^{\lambda_{k=1}}(\alpha_kP_{k-1})^{e^{x_\ell\beta}}=$$

$$\prod_{j=1}^{k}\prod_{\ell\in C_j\cup D_j}(\alpha_1\alpha_2\cdots\alpha_{j-1})^{e^{x_\ell\beta}}\prod_{\ell\in D_j}(1-\alpha_j^{e^{x_\ell\beta}})\prod_{\ell=1}^{\lambda_{k+1}}(\alpha_kP_{k-1})^{e^{x_\ell\beta}}=$$

$$\prod_{j=1}^{k=1}\prod_{\ell\in D_j}(1-\alpha_j^{e^{x_\ell\beta}})\prod_{\ell\in R_j-D_j}\alpha_j^{e^{x_\ell\beta}},$$

where R_j equals the risk set at time t_{j-1}. D_{k+1} is the empty set.

$$\frac{d\log L}{d\,\alpha_j}=0\Rightarrow\frac{-\sum_{\ell\in D_j}e^{x_\ell\beta}\alpha_j^{e^{x_\ell\beta-1}}}{1-\alpha_j^{e^{x_\ell\beta}}}+\sum_{\ell\in R_j-D_j}\frac{e^{x_\ell\beta}}{\alpha_j}=0.$$

The expression

$$\frac{\sum_{\ell\in D_j}e^{x_\ell\beta}\alpha_j^{e^{x_\ell\beta-1}}}{1-\alpha_j^{e^{x_\ell\beta}}}=\sum_{\ell\in R_j-D_j}\frac{e^{x_\ell\beta}}{\alpha_j}$$

needs to be solved numerically for $\alpha_1,\alpha_2,...,\alpha_k$. The last term needs to be proven on the exam. But it does simplify in special cases.

1. If $d_j = |D_j| = 1$, then ℓ becomes j and

$$\frac{e^{x_j\beta}}{1-\alpha_j^{x_j\beta}} = \sum_{\ell \in R_j} e^{x_\ell \beta} \Rightarrow \alpha_j = \frac{\log\left\{1-e^{x_j\beta}\right\}}{\frac{\sum_{\ell\in R_j} e^{x_\ell\beta}}{e^{x_j\beta}}}.$$

   Initial values for α_j in the general case use $\alpha_j^{e^{x_\ell\beta}} \approx 1 + (\log \alpha_j)e^{x_\ell\beta}$ because $a^b \approx e^{b\log a} = 1 + b\log a]$.

2. Suppose there are only two populations. $d_j = d_{1j} + d_{2j}$. $R_j = n_{1j} + n_{2j}$. Then, $x = 0$ or $x = 1$. Then,

$$s(t|x) = \begin{cases} s_0(t), & x = 0 \\ [s_0(t)]^{e^\beta} & x = 1 \end{cases}$$

   Then, $\frac{d_{1j}}{1-\alpha_j} + \frac{d_{2j}e^\beta}{1-\alpha_j^{e^\beta}} = n_{1j} + n_{2j}e^\beta$. Also, $\sum_{\ell\in R_j} 1 = n_{1j}$ for $x = 0$. Solve numerically for α_j. Further, suppose there are no ties. Then, $d_j = 1 \Rightarrow d_{1j} + d_{2j} = 1$. $d_{1j} = 0$ and $d_{2j} = 1 \Rightarrow$

$$\frac{e^\beta}{1-\alpha_j^{e^\beta}} = n_{1j} + n_{2j}e^\beta = \alpha_j = 1 - \frac{e^\beta}{n_{1j}+n_{2j}e^\beta} \Rightarrow \alpha_j = 1 - \frac{1}{n_{1j}+n_{2j}e^\beta}.$$

   $s_0(t_j) = \alpha_1\alpha_2\cdots\alpha_j$. Then, $\widehat{s}_0(t_j) = \widehat{\alpha}_1\widehat{\alpha}_2\cdots\widehat{\alpha}_j$.

$$\widehat{s}(t|x) = \begin{cases} \widehat{s}_0(t), & x = 0 \\ [\widehat{s}_0(t)]^{e^\beta} & x = 1 \end{cases}$$

   In general, $\widehat{s}_0(t_j) = \widehat{\alpha}_1\widehat{\alpha}_2\cdots\widehat{\alpha}_j$ and $\widehat{s}(t_j|x_\ell) = (\widehat{\alpha}_1\widehat{\alpha}_2\cdots\widehat{\alpha}_j)^{e^{x_\ell\beta}} = [s_0(t_j)]^{e^{x_\ell\beta}}$.

3. Another estimator comes from Breslow (1974),

$$\widehat{H}_0(t) = \sum_{j:t_j\le t} \frac{d_j}{\sum_{\ell in R_j} e^{x_\ell\beta}}.$$

   If there are no covariates, $\widehat{H}_0(t) = \frac{d_j}{n_j}$ for $x_\ell = 0$. Solve $-\log(1-\widehat{s}_0(t)) = \widehat{H}_0(t)$ for $\widehat{s}_0(t)$. Then, obtain $1 - \widehat{s}_0(t) = e^{-\widehat{H}_0(t)} \Rightarrow \widehat{s}_0(t) = 1 - e^{-\widehat{H}_0(t)}$. If all $d_j = 1$ (no ties), then this estimator is very close to the mle.

16.8 Review of Statistical Tests and Distributions for Survival Analyzes

16.8.1 Cox-Mantel Test

This test is covered on pages 107-108 of the test book. The hypothesis is $H_0 : s_1(t) = s_2(t)$. This is the same as testing $H_0 : \beta = 0$ in the Cox proportional hazard model. The data comes in times t_i and deaths d_i, $t_1, t_2, ..., t_k$; $d_1, d_2, ..., d_k$. $d_i = d_{1i} + d_{2i}$. $n_i = n_{1i} + n_{2i}$.

16.8.2 Log-Rank Test

This is the log-rank test of Mantel (1966). The null hypothesis is $H_0 : s_1(t) = s_2(t)$. $\widehat{s}(t) = \prod_{j:j\leq t}\left(1 - \frac{d_j}{r_j}\right)$ where r_j equals the risk set at time $t_j = r_{1j} + r_{2j}$ and $d_j = d_{1j} + d_{2j}$. $\log(\widehat{s}(t)) = \sum \log\left(1 - \frac{d_j}{r_j}\right) = -\sum \frac{d_j}{r_j} + \Theta\left(\frac{1}{r_j^2}\right)$. The scores for the test are $w_i = 1 - e(t_i)$ for uncensored observations at time t_i where $e(t_i) = \sum_{i:t_j\leq t_i} \frac{d_j}{r_j}$. Ignore the $\Theta\left(\frac{1}{r_j^2}\right)$ terms. $w_i = -e(t_j)$ for censored observations where t_j^+ is the death time less than or equal to t_i and closest to t_i. $\sum_{i=1}^n w_i = 0$, $n = n_1 + n_2$. s equals to the sum of the scores from one group. $E(w_i|\underline{w}) = 0$ under H_0. Also, $Var(w_i|\underline{w}) = \sum \frac{w_i^2}{n}$. $E(s|\underline{w}) = 0$. $Var(s|\underline{w}) = \frac{\sum d_j(r_j-d_j)(n_1n_2}{r_j(n_1+n+2)(n_1+n_2-1)} = n_1n_2 \sum \frac{w_i^2}{n(n-1)}$, where $r_j = n_{1j} + n_{2j}$. $z = \frac{s}{\sqrt{Var(s|\underline{w})}} \to N(0,1)$. Suppose that we test $H_1 : s_1 > s_2$. s equals the sum of scores for group 1. We calculate $1 + \log s_1(t_i)$ and $1 + \log s_2(t_i)$. Scores from group 1 tend to be smaller than group 2 if H_1 is true. Reject H_0 if $z < -z_\alpha$.

16.8.3 Chi-Square Test

The data comes in the form.

t_1	t_2	$\cdots$	t_i	$\cdots$	t_k	
d_1	d_2	$\cdots$	d_i	$\cdots$	d_k	deaths
n_1	n_2	$\cdots$	n_i	$\cdots$	n_k	risk sets

We test $H_0 : s_1(t) = s_2(t)$ where $d_i = s_{1i} + d_{2i}$ and $n_i = n_{1i} + n_{2i}$. At time t_i, given d_i, n_{1i}, n_{2i}, if H_0 is true, then $E(d_{1i}) = \frac{n_{1i}}{n_{1i}+n_{2i}} d_i = e_{1t_i}$ and $e_1 = \sum_{i=1}^k e_{1t_i}$ and $o_1 = \sum_{i=1}^k d_{1i}$. The statistic $x^2 = \frac{(o_1-e_1)^2}{e_1} + \frac{(o_2-e_2)^2}{e_2} \to \chi^2(1)$. $E(Q_1) = e_1$, o_1 equals the observed deaths from group 1.

16.8.4 Cox's $F-$Test

This test is Cox's $F-$Test from Cox (1964). Assume no censoring. Then, $s_i(t) = e^{-\frac{t}{\theta_i}}$, $i = 1, 2$. $H_0 : s_1(t) = s_2(t) \Rightarrow \theta_1 = \theta_2$. From a sample of size n, from $\exp\{\theta\}$, let x_r be the r^{th} order statistic. Then,

$$E(x_r) = \left(\frac{1}{n} + \frac{1}{n-1} + \cdots + \frac{1}{n-r+1}\right)\theta.$$

$n = n_1 + n_2$ and $t_1 < t_2 < \cdots < t_n$. The scores are $t_{r_n} = \frac{1}{n} + \frac{1}{n-1} + \cdots + \frac{1}{n-r+1}$, $r = 1, 2, ..., n$. Then, find $\bar{t}_1$ equal to the average of scores of observations from group 1 and $\bar{t}_2$ equal to the average of scores of observations from group 2. The the test statistic is $f = \frac{\bar{t}_1}{\bar{t}_2} \approx F(2n_1, 2n_2)$. This is due to the following result about exponentials. Suppose we are given two samples from two exponential distributions. $x_1, x_2, ..., x_{n1} \sim \exp(\theta_1)$ and $y_1, y_2, ..., y_{n2} \sim \exp(\theta_2)$. If we wish to test the null hypothesis $H_0 : \theta_1 = \theta_2 = \theta$, then $\frac{\bar{x}}{\bar{y}} \sim F(2n_1, 2n_2)$. Suppose the alternative hypothesis is $H_1 : s_1 > s_2$. Then that implies that $\theta_1 > \theta_2$ because $s_i(t) = e^{-\frac{t}{\theta_i}}$ is an increasing function of θ_i. Note that $\log s_i(t) = -\frac{t}{\theta_i}$ is increasing. Reject H_0 if $f > F_\alpha(2n_1, 2n_2)$. For *singly censored data,* assume a fixed censored time T for both groups. There are p death times. $t_1, t_2, ..., t_p$ are the ordered death times. If $p = d_1 + d_2$ and $n = n_1 + n_2$, then $n_1 - d_1$ from group 1 are censored observations. t_r $r = 1, 2, ..., p$ are given scores. The score for t_r is t_{r_n}. The score of all of the censored observations are given the same score $t_{p+1,n}$. $\bar{t}_1 = \frac{d_1 d_1' + (n_1-d_i)p_{p+1,n}}{d_1}$. Now, $f = \frac{\bar{t}_1}{\bar{t}_2} \approx F(2d_1, 2d_2)$. Here are some comments on the tests for $s_1(t) = s_2(t)$.

1. V of the Cox-Mantel test is the same as S of the log −rank test if S is based on scores of group 2.
2. For small sample sizes ($n_1 < 50$, $n_2 < 50$), Gehan & Thomas (1969) show that Cox's $F-$Test is more powerful than Gehan's Generalized Wilcoxon Test if the samples are from exponential or Weibull distributions.

3. When the survival functions cross, none of the tests considered here are powerful. Consider H_0 : $s_1(t) = s_2(t)$ versus $H_1 : s_1(t) \neq s_2(t)$. There are no powerful tests for this either.

The test in this section is also closely related to the Savage exponential test. Reference Lehmann, E. L. and D'Abrera, H. J. M. (1975), *Nonparametrics, Statistical Methods Based on Ranks,* Holden-Day, Inc., Oakland, California, p 104.

16.8.5 Mantel and Hanzel Test

The Mantel and Hanzel test is meant for testing about two stratified groups simultaneously. s equals to the number of strata and it is the same for both groups. n_{ji} equals to the number in group j and strata i. $j = 1, 2$; $i = 1, 2, ..., s$. d_{ji} equals to the number of deaths in the $(j, i)^{th}$ cell.

	Deaths	Survivors	Total
Group 1	d_{1i}	$n_{1i} - d_{1i}$	n_{1i}
Group 2	d_{2i}	$n_{2i} - d_{2i}$	n_{2i}
Total	D_i	S_i	T_i

Test $p_{ij} = P(\text{death } | \text{group } j, \text{ strata } i)$. $H_0 : p_{i1} = p_{i2}$, $i = 1, 2, ..., s$. Given H_0, D_i, T_i, n_{1i}, and n_{2i} we have a hyper-geometric distribution for d_{1i} is

$$\frac{\begin{pmatrix} D_i \\ d_{1i} \end{pmatrix} \begin{pmatrix} s_i \\ n_{1i} - d_{1i} \end{pmatrix}}{\begin{pmatrix} T_i \\ n_{1i} \end{pmatrix}}.$$

The conditional mean and variance are $E(d_{1i}) = \frac{n_{1i}}{T_i} \times D_i$,

$$Var(d_{1i}) = \frac{n_{1i} n_{2i} D_i s_i}{T_i^2 (T_i - 1)}.$$

$$\frac{\left[\sum_{i=1}^{s} d_{1i} - \sum_{i=1}^{s} E(d_{1i})\right]^2}{\left[\sum_{i=1}^{s} d_{1i}\right]^{\frac{1}{2}}} \to \chi^2(1).$$

What is the distribution of the following expression? It is not the same.

$$\sum_{i=1}^{s} \frac{(d_{1i} - E(d_{1i}))^2}{\sqrt{Var(d_{1i})}}.$$

16.8.6 Other-Than Linear Distributions

October 11, 1997. Lecture 11 is missing.

For the exponential function, $\log s(t) = -\lambda t$ is linear. But for other-than linear functions, $\log s(t) = -(\lambda t)^\delta$, $\delta > 0$. $s(t) = e^{-(\lambda t)^\delta}$, $F(t) = 1 - e^{-(\lambda t)^\delta}$, $f(t) = \lambda \delta (\lambda t)^{\delta - 1} e^{-(\lambda t)^\delta}$, $t > 0$, $\lambda, \delta > 0$. The Weibull distribution is $h(t) = \frac{f(t)}{s(t)} = \lambda \delta (\lambda t)^{\delta - 1}$ where λ is the scale parameter and δ is the shape parameter.

$$\mu = E(T) = \frac{\Gamma\left(1 + \frac{1}{\delta}\right)}{\lambda}, \ \ \sigma^2 = Var(T) = \frac{1}{\lambda^2}\left[\Gamma\left(1 + \frac{2}{\delta}\right) - \Gamma\left(1 + \frac{1}{\delta}\right)\right].$$

Let $x = T^\delta$, $x \sim \exp(\lambda^\delta) = \exp(\lambda^*)$. The *delayed Weibull distribution* will be covered next. If $X = T - G$ is Weibull, then T is a delayed Weibull distribution with support (G, ∞). Now, the distribution of X has three parameters.

Example: Consider example 6.2 on page 138-139 of the text book. There are two groups exposed to carcinogen DMBA. $\widehat{s}(t)$ is plotted using the Kaplan-Meir estimators and again for the delayed Weibull estimators. $\widehat{s}_2(t) > \widehat{s}_1(t)$.

How do we find the estimator of G? Consider the trial times $t_1, t_2^+, ..., t_n$. Then, $T \geq G$. The mle for T is $t_{(1)}$, the smallest observation. $t_{(1)} \geq G$, $E(t_{(1)} - G) \geq 0$, $t_{(1)}$ has positive bias.

Consider the log normal distribution. T is said to have the log normal distribution if $X = \log T \sim N(\mu, \sigma^2)$. The pdf is given by

$$f(t) = \frac{1}{t\sigma\sqrt{2\pi}} \exp\left\{-\frac{1}{2\sigma^2}(\log t - \mu)^2\right\}, t > 0,\ -\infty < \mu < \infty,\ \sigma > 0.$$

Consider the transformation $X = logt$. $dx = \frac{1}{t}\, dt$.

$$f(t)\, dt = \frac{1}{\sqrt{2\pi}\sigma} \exp\left\{-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right\} dx,\ -\infty < x < \infty$$

and $s(t) = 1 - \Phi\left(\frac{\log at}{\sigma}\right)$ where $a = e^{-\mu}$. $\Phi(z)$ is the distribution function of the standard normal. $M_T^{(\mu)} = E(e^{\mu T}) = \cdots \Rightarrow -M_x^{(\mu)} = E(e^{\mu x}) = e^{\mu u + \frac{1}{2}\sigma^2 u^2}$, $T = e^x$. $E(T) = E(e^x) = \mu_x(1) = e^{\mu + \frac{1}{2}\sigma^2}$. $E(T^2) = \mu_x(2)$. $\sigma_T^2 = e^{2\mu+\sigma^2}(e^{\sigma^2} - 1)$. The median is $median(T) = e^{\mu}$. The mode is $mode(T) = e^{\mu - \sigma^2}$. For the estimation of μ_T, σ_T^2, etc look at the data. For the data $t_1, t_2, ..., t_n$, look at $X = \log T$. For the data $x_1, x_2, ..., x_n$, it has a normal distribution. Then, $\widehat{\mu} = \bar{x}$ and $\widehat{\sigma}^2 = s^2 = \frac{1}{n}\sum(x_i - \bar{x})^2$. If $\widehat{\theta}$ is the mle of θ, then $\Phi(\widehat{\theta})$ is the mle of Φ, if it is a one-to-one function of θ. $\frac{T - \mu_T}{\sigma_T} \to N(0,1)$ as $\sigma \to 0$. $h(t) = \frac{f(t)}{1 - \Phi\left(\frac{\log at}{\sigma}\right)}$. Using probability graph paper, if $(F(t), t)$ is plotted, then it is linear on this type of paper.

Example: This is the example on page 144-145 of the text book. It is leukemia survival data from 1943-1952. $(F_n(t), t)$ is plotted on probability graph paper. T equals to the survival time from diagnosis to the death in months. The delayed log-normal distribution ($G = 4$) is linear.

Consider the gamma distribution.

$$f(t) = \frac{\lambda}{\Gamma(\delta)}(\lambda t)^{\delta-1} e^{-\lambda t}, t > 0,\ \lambda,\ \delta > 0.$$

$$F(t) = \int_0^t \frac{\lambda}{\Gamma(\delta)}(\lambda u)^{\delta-1} e^{-\lambda u}\, du = \int_0^{\lambda t} \frac{1}{\Gamma(\delta)} e^{-x} x^{\delta-1}, dx$$

is called the *incomplete gamma function* because $\Gamma(a) = \int_0^\infty e^{-x} x^{a-1}, dx$. $h(t) = \frac{f(t)}{1-F(t)}$. For $\delta = n$, an integer, then $F(t) = 1 - \sum_{k=0}^{n-1} e^{-\lambda t}\frac{(\lambda t)^k}{k!}$. $P(T \leq t) = P(X \geq n)$, $X \sim Poisson(\lambda t)$. If $x_1, x_2, ..., x_n$ are iid $\exp(\lambda)$, then $y = \sum_{i=1}^n x_i \sim gamma(\lambda, n)$.

16.8.7 Other Distributions

For the exponential distribution $h(t) = \lambda$. Taking $h(t)$ as a linear function, $h(t) = \lambda + \delta t$ for $\lambda > 0$. $\delta < 0$ is only possible if T has a finite support since $h(t)$ cannot be negative. Find $s(t)$. $H(t) = \int_0^t h(u)\, du = \lambda t + \frac{\delta t^2}{2} \Rightarrow s(t) = e^{-H(t)} = e^{-\lambda t - \frac{\lambda t^2}{2}} \Rightarrow F(t) = 1 - s(t) \Rightarrow f(t) = \frac{d\,F(t)}{dt}$.

16.8.8 Gompers Distribution

$h(t) = \exp(\lambda + \delta t)$. $H(t) = \int_0^t h(u)\,du = \exp(\lambda)\frac{(\exp(\lambda t)-1)}{\delta} = \frac{e^{\lambda}(e^{\lambda t}-1)}{\delta}$. The hazard rate as a step function is

$$h(t) = \begin{cases} a_1, & 0 < t < t_1 \\ a_2, & t_1 < t < t_2 \\ \vdots & \\ a_k, & t_k \geq t_{k-1} \end{cases}$$

16.9 Homework and Answers

1. Let T, the survival time, be $\exp(\lambda)$ for a given λ and let $\lambda \sim gamma(\alpha, k)$ where $\alpha > 0, k > 0$. Find the hazard rate $h(t)$ for the unconditional distribution of T and show that it is monotone decreasing. Here $E(T|\lambda) = \frac{1}{\lambda}$. Solution:

$$g(\lambda) = \frac{1}{\Gamma(\alpha)k^{\alpha}}\lambda^{\alpha-1}e^{-\frac{\lambda}{k}}.$$

First find $f(T, \lambda, \alpha, k)$:

$$f(T,\lambda,\alpha,k) = f(T|\lambda)g(\lambda) = \lambda e^{-\lambda T}\frac{1}{\Gamma(\alpha)k^{\alpha}}\lambda^{\alpha-1}e^{-\frac{\lambda}{k}} = \frac{1}{\Gamma(\alpha)k^{\alpha}}\lambda^{\alpha}e^{-(\lambda T+\frac{\lambda}{k})} = \frac{1}{\Gamma(\alpha)k^{\alpha}}\lambda^{\alpha}e^{-\lambda(T+\frac{1}{k})}.$$

Need to find $f_1(T)$.

$$f_1(T) = \int_0^{\infty} f(T,\lambda,\alpha,k)d\lambda = \int_0^{\infty}\frac{1}{\Gamma(\alpha)k^{\alpha}}\lambda^{\alpha}e^{-\lambda(T+\frac{1}{k})}\,d\lambda$$

Substitute $\beta' = \frac{1}{\frac{1}{T+\frac{1}{k}}}$ and $\alpha' = \alpha + 1$. This yields

$$\frac{\Gamma(\alpha+1)}{\Gamma(\alpha)k^{\alpha}\left(T+\frac{1}{k}\right)^{\alpha+1}}\overbrace{\int_0^{\infty}\frac{\left(T+\frac{1}{k}\right)^{\alpha+1}\lambda^{\alpha-1}e^{-\lambda(T+\frac{1}{k})}}{\Gamma(\alpha+1)}d\lambda}^{=1 \text{ (gamma pdf)}} = \frac{\Gamma(\alpha+1)}{\Gamma(\alpha)k^{\alpha}\left(T+\frac{1}{k}\right)^{\alpha+1}} = \frac{\alpha}{k^{\alpha}\left(T+\frac{1}{k}\right)^{\alpha+1}}.$$

Need to find $F_1(T)$.

$$F_1(T) = \int_0^T f_1(x)\,dx = \frac{\alpha}{k^{\alpha}}\int_0^T\left(x+\frac{1}{k}\right)^{-\alpha-1}dx = \frac{\alpha}{k^{\alpha}}\left[-\frac{\left(x+\frac{1}{k}\right)^{-\alpha}}{\alpha}\right]_0^T = -\frac{\left(T+\frac{1}{k}\right)^{-\alpha}}{k^{\alpha}} + \frac{\left(\frac{1}{k}\right)^{-\alpha}}{k^{\alpha}} =$$

$$-\frac{\left(T+\frac{1}{k}\right)^{-\alpha}}{k^{\alpha}} + 1 = -\frac{1}{k^{\alpha}\left(T+\frac{1}{k}\right)^{\alpha}} + 1 = F_1(T).$$

The hazard function is

$$h(t) = \frac{f_1(t)}{1-F_1(t)} = \frac{\frac{\alpha}{k^{\alpha}\left(T+\frac{1}{k}\right)^{\alpha+1}}}{1+\frac{1}{k^{\alpha}\left(T+\frac{1}{k}\right)^{\alpha}}-1} = \frac{\frac{\alpha}{k^{\alpha}\left(T+\frac{1}{k}\right)^{\alpha+1}}}{\frac{1}{k^{\alpha}\left(T+\frac{1}{k}\right)^{\alpha}}} = \frac{\alpha}{T+\frac{1}{k}}.$$

Note that $\alpha, k, T > 0$. Then, $h(t)$ is a decreasing function for all T for fixed α and k. $h(0) \neq h(t_1) \neq \cdots \neq h(t_n)$ for any t. Thus, $h(t)$ is monotone.

2. Let T be a continuous random variable with survival function $s(t)$. The mean residual life function $M(t)$ is defined as $M(t) = E(T|T \geq t) - t$.

   (a) Prove that $M(t) = \int_t^\infty s(x)\,dx/s(t)$. Also, obtain $s(t)$ in terms of $M(t)$ showing that $M(t)$ uniquely defines the distribution of T. Solution:

$$\int_t^\infty s(x)\,dx = xs(x)\Big|_t^\infty + \int_t^\infty xf(x)\,dx.$$

   Consider $xs(x)\Big|_t^\infty$. $\lim_{x\to\infty} x[1-F(x)] = 0$. proof: If $E(x) < \infty$, then $\lim_{t\to\infty}\int_t^\infty xf(x)\,dx = 0$ because $E(x) = \underbrace{\int_0^t xf(x)\,dx}_{=\mu \text{ as } t\to\infty} + \underbrace{\int_t^\infty xf(x)\,dx}_{\text{must be } 0}$. $\int_t^\infty xf(x)\,dx \geq \int_t^\infty tf(x)\,dx = t[1-F(t)] \Rightarrow \lim_{t\to\infty} t[1-F(t)] = 0$. So, we can conclude that $\int_t^\infty s(x)\,dx = -ts(t) + \infty_t^\infty\,dx$. $\int_t^\infty \frac{s(x)\,dx}{s(t)} = \int_t^\infty \frac{xf(x)\,dx}{s(t)} - t = m(t) = E(T|T>t) - t$.

   Prove that:

$$\lim_{t\to\infty} dtM(t) = dt_{t\to\infty}\left(\frac{d}{dt}\log f(t)\right)^{-1}$$

   where $f(t) = -s'(t)$. Solution: Using L'Hopital's rule,

$$\lim_{t\to\infty}\frac{\int_t^\infty s(x)\,dx}{s(t)} = \lim\frac{-s(t)}{-f(t)}.$$

   Using L'Hopital's rule again,

$$\lim\frac{-f(t)}{f'(t)} = \lim\left[\frac{-d}{dt}\log f(t)\right]^{-1}$$

3. The distribution with $h(t)$ is non-decreasing for $t \geq 0$ is known as an increasing failure rate (IFR) distribution. Also, if $H(t)/t$ is non-decreasing for $t > 0$, then it is known as an increasing failure rate on the average (IFRA). Prove that IFR $\Rightarrow$ IFRA. If $h(t) \uparrow t$, then prove $\frac{H(t)}{t} \uparrow t$. Let $g(t) = \frac{H(t)}{t}$. Take the derivative $\frac{dg(t)}{dt} = \frac{th(t)-H(t)}{t^2}$. $H(t) = \int_0^t h(x)\,dx \leq th(t) \Rightarrow \frac{dg}{dt} > 0 \Rightarrow g(t) \uparrow t$.

4. Consider the following two estimates for the hazard function $h(t)$ at the midpoint of the interval (t_{i-1}, t_i).

$$\widehat{h}(t_{mi}) = \frac{2\widehat{q}_i}{b_i(1+\widehat{p}_i)} \text{ and } \tilde{h}(t_{mi}) = -\log\frac{\widehat{p}_i}{b_i}.$$

   (a) Compare the two estimators by expanding them in powers of $\widehat{q}_i$.

$$\tilde{h}(t_{mi}) = -\frac{\log\widehat{p}_i}{b_i} = -\frac{\log(1-\widehat{q}_i)}{b_i} = \frac{\widehat{q}_i + \frac{\widehat{q}_i^2}{2} + \frac{\widehat{q}_i^3}{3} + \cdots}{b_i}.$$

$$\widehat{h}(t_{mi}) = \frac{2}{b_i}\left[-1+1+\frac{1}{2}\widehat{q}_i + \left(\frac{1}{2}\widehat{q}_i\right)^2 + \left(\frac{1}{2}\widehat{q}_i\right)^3 + \cdots\right] = \frac{2}{b_i}\left[\frac{1}{2}\widehat{q}_i + \left(\frac{1}{2}\widehat{q}_i\right)^2 + \left(\frac{1}{2}\widehat{q}_i\right)^3 + \cdots\right] =$$

$$\frac{1}{b_i}\left[\widehat{q}_i + \frac{\widehat{q}_i^2}{2} + \frac{\widehat{q}_i^3}{4} + \cdots\right].$$

Ignoring terms $\Theta(\widehat{q}_i^3)$, the two estimators are the same.

(b) Derive estimates for the asymptotic variance of these estimators.

$$\widehat{h}(t_{mi}) = \frac{2\widehat{q}_i}{b_i(2-\widehat{q}_i)},$$

$$\frac{d\,\widehat{h}(t_{mi})}{d\,\widehat{q}_i} = \frac{2}{b_i(2-\widehat{q}_i)} - \frac{2\widehat{q}_i}{b_i(2-\widehat{q}_i)^2} = \frac{\widehat{h}(t_{mi})}{\widehat{q}_i} - \frac{b_i\widehat{h}^2(t_{mi})}{2\widehat{q}_i}.$$

$$Var[\widehat{h}(t_{mi})] = \left[\frac{\widehat{h}(t_{mi})}{\widehat{q}_i} - \frac{b_i\widehat{h}^2(t_{mi})}{2\widehat{q}_i}\right]^2 Var(\widehat{q}_i) =$$

$$\frac{\widehat{h}(t_{mi})^2\widehat{q}_i\widehat{p}_i}{\widehat{q}_i^2 n_i}\left[1 - \frac{b_i\widehat{h}(t_{mi})}{2}\right]^2 = \frac{\widehat{h}(t_{mi})^2\widehat{p}_i}{\widehat{q}_i n_i}\left[1 - \frac{b_i\widehat{h}(t_{mi})}{2}\right]^2.$$

Working with the second estimator,

$$\frac{d\,\tilde{h}(t_{mi})}{d\,\widehat{p}_i} = -\frac{1}{\widehat{p}_i b_i}.$$

The variance is

$$\left(-\frac{1}{\widehat{p}_i b_i}\right)^2 \frac{\widehat{p}_i\widehat{q}_i}{n_i} = \frac{\widehat{q}_i}{\widehat{p}_i b_i^2 n_i}$$

Since $Var(\tilde{h}) - Var(\widehat{h}) > 0$, $Var(\tilde{h})$ is larger.

5. Let the survival time T have the pdf $f(x)$, $x > 0$. We put n items on test and stop the experiment whenever both r fixed failures and the T time on the test are achieved. Derive the likelihood function for their data. Solution: Stop when at least r failures and at least time T for the test has been reached. Let k equal to the number of failures in $(0,T)$. If $k > r$, we stop at time T. If $k < r$, we stop at the r^{th} failure. Case 1: For $k \geq r$, the data is $(t_1, t_2, ..., t_k, k)$ and $t_1 < t_2 < \cdots < t_k$. The likelihood function is

$$L = P(t_1, t_2, ..., t_k, k) = P(k)P(t_1, t_2, ..., t_k|k) = \begin{pmatrix} n \\ k \end{pmatrix} f(T)^k[1-F(T)]^{n-k}.$$

$$P(t_1, t_2, ..., t_k|k) = \frac{f(t_1)}{F(t)}\frac{f(t_2)}{F(t)}\cdots\frac{f(t_k)}{F(t)}k!$$

Then,

$$L = \frac{n!}{(n-k)!}f(t_1)f(t_2)\cdots f(t_k)[1-F(T)]^{n-k},\ k = r, r+1, ...$$

Case 2: For $k < r$, $t_1 < t_2 < \cdots < t_k < T < t_{k+1} < \cdots < t_r$. The likelihood function is

$$L = \begin{pmatrix} n \\ k \end{pmatrix} F(t)^k[1-F(T)]^{n-k}\frac{f(t_1)f(t_2)\cdots f(t_k)}{F(T)^k}k!\begin{pmatrix} n-k \\ r-k \end{pmatrix}\left[\frac{F(t_r)-F(T)}{1-F(T)}\right]^{r-k}\left[\frac{1-F(t_r)}{1-F(T)}\right]^{n-r}\times$$

$$\frac{f(t_{k+1})\cdots f(t_r)}{[F(t_r)-F(t)]^{r-k}}(r-k)! = \frac{n!}{(n-r)!}f(t_1)f(t_2)\cdots f(t_k)t(t_{k+1})\cdots f(t_r)[1-F(t_r)]^{n-r}.$$

6. Using the notation in Lecture 3, prove that $Cov(\widehat{P}_j, \widehat{P}_\ell) = (1 - P_j)P_\ell/n,\ j < \ell$. Solution: Note $n_{i+1} \sim binomial(n, P_i)$. For $j < \ell$, $(n_{\ell+1}, n_{j+1} - n_{\ell+1}) \sim trinomial(n, P_{\ell 1}, P_j - P_\ell)$. $Cov(\widehat{P}_j, \widehat{P}_\ell) = Cov\left(\frac{n_{j+1}}{n}, \frac{n_{\ell+1}}{n}\right) = \frac{1}{n^2}Cov(n_{j+1} - n_{\ell+1} + n_{\ell+1}, n_{\ell+1}) = \frac{1}{n^2}Var(n_{\ell+1}) + Cov(n_{\ell+1}, n_{j+1} - n_{\ell+1}) = \frac{1}{n^2}[nP_\ell(1 - P_\ell) - nP_\ell(P_j - P_\ell)] = \frac{1}{n}P_\ell(1 - P_\ell)$.

7. Using the notation in Lecture 6, derive $\widehat{V}(\widehat{f}(t_{mi}))$. Solution: $\widehat{f}(t_{m_i}) = \frac{\widehat{p}_1 \cdots \widehat{p}_{i-1}(1-\widehat{p}_i)}{b_i} = g(\underline{\widehat{p}})$. $g(f) = \frac{p_1 \cdots p_{i-1}(1-p_i)}{b_i}$. $\frac{d\,g}{d\,p_j} = \frac{p_1 \cdots p_{j-1}p_{j+1} \cdots p_{i-1}(1-p_i)}{b_i} = \frac{g(\underline{p})}{p_j}, j < i$. $\frac{d\,g}{d\,p_i} = \frac{-g(\underline{p})}{1-p_i}$. Note $Cov(\widehat{p}_j, \widehat{p}_\ell) = 0$. $Var(\widehat{f}(t_{mi})) = \sum_{j=1}^{i} Var(\widehat{p}_j)\left(\frac{d\,g}{d\,p_j}\right)^2 = g^2(\underline{p})\left[\sum_{j=1}^{i-1}\frac{q_j}{n_j p_j} + \frac{p_i}{n_i q_i}\right]$.

8. Do exercise 2.2 on page 17 of the text book.

Interval	$\widehat{s}(t)$	$\widehat{f}(t)$	$\widehat{h}(t) = \frac{\widehat{f}(t)}{\widehat{s}(t)}$
$0-1$	1.0	0.02593	0.02593
$1-5$	0.974	0.000818	0.00084
$5-10$	0.96998	0.000466	0.00048
$10-15$	0.96765	0.000428	0.00044
$15-20$	0.96551	0.00088	0.00091
$20-25$	0.96111	0.001188	0.00124
$25-30$	0.95517	0.001224	0.00128
$30-35$	0.94905	0.001522	0.00160
$35-40$	0.94144	0.00216	0.00229
$40-45$	0.93064	0.003372	0.0036
$45-50$	0.91378	0.005244	0.0057
$50-55$	0.88756	0.00809	0.00911
$55-60$	0.84711	0.011288	0.1333
$60-65$	0.79067	0.01584	0.02003
$65-70$	0.71147	0.02058	0.02893
$70-75$	0.60857	0.025374	0.04169
$75-80$	0.48170	0.029188	0.06060
$80-85$	0.33576	0.030068	0.08956
85^+	0.18542	$--$	$--$

9. Do exercise 4.1 on page 101 of the text book. For treatment 1,

Survival Time	$\widehat{S}(t)$	i	r
3.9	$\frac{10}{11}$	1	1
5.4	$\frac{10}{11} \times \frac{9}{10} = \frac{9}{11}$	2	2
7.9	$\frac{9}{11} \times \frac{8}{9} = \frac{8}{11}$	3	3
10.5	$\frac{8}{11} \times \frac{7}{8} = \frac{7}{11}$	4	4
16.6^+	$--$	5	$--$
16.9^+	$--$	6	$--$
17.1^+	$--$	7	$--$
19.5	$\frac{7}{11} \times \frac{3}{4} = \frac{21}{44}$	8	8
23.8^+	$--$	9	$--$
33.7^+	$--$	10	$--$
33.7^+	$--$	11	$--$

The time of 19.5 does not agree with the text book on page 21. The variances are calculated with the formula $\widehat{Var}(\widehat{s}(t)) = [\widehat{s}(t)]^2 \sum_r \frac{1}{(n-r)(n-r+1)}$.

$$\widehat{Var}(\widehat{s}(3.9)) = \left(\frac{10}{11}\right)^2 \left[\frac{1}{10(11)}\right] = 0.00751.$$

$$\widehat{Var}(\widehat{s}(5.4)) = \left(\frac{9}{11}\right)^2 \left[\frac{1}{10(11)} + \frac{1}{9(10)}\right] = 0.01352.$$

$$\widehat{Var}(\widehat{s}(7.9)) = \left(\frac{8}{11}\right)^2 \left[\frac{1}{10(11)} + \frac{1}{9(10)} + \frac{1}{8(9)}\right] = 0.01803.$$

$$\widehat{Var}(\widehat{s}(10.5)) = \left(\frac{7}{11}\right)^2 \left[\frac{1}{10(11)} + \frac{1}{9(10)} + \frac{1}{8(9)} + \frac{1}{7(8)}\right] = 0.02104.$$

$$\widehat{Var}(\widehat{s}(19.5)) = \left(\frac{21}{44}\right)^2 \left[\frac{1}{10(11)} + \frac{1}{9(10)} + \frac{1}{8(9)} + \frac{1}{7(8)} + \frac{1}{3(4)}\right] = 0.03082.$$

The median m for treatment 1 is between the two observations as follow. We must use uncensored observations.

t	$\widehat{s}(t)$
10.5	$\frac{7}{11}$
m	0.5
19.5	$\frac{21}{44}$

For treatment 2,

Survival Time	$\widehat{S}(t)$	i	r
6.9	$\frac{18}{19}$	1	1
7.7	$\frac{18}{19} \times \frac{17}{18} = \frac{17}{19}$	2	2
7.8^+	$--$	3	$--$
8.0	$\frac{17}{19} \times \frac{15}{16} = \frac{255}{304}$	4	4
8.2^+	$--$	5	$--$
8.2^+	$--$	6	$--$
8.3	$\frac{255}{304} \times \frac{12}{13} = \frac{3060}{3952}$	7	7
10.8^+	$--$	8	$--$
11.0^+	$--$	9	$--$
12.2^+	$--$	10	$--$
12.5^+	$--$	11	$--$
14.8^+	$--$	12	$--$
16.0^+	$--$	13	$--$
18.1^+	$--$	14	$--$
21.4^+	$--$	15	$--$
23.0^+	$--$	16	$--$
24.4	$0.774 \times \frac{2}{3} = 0.516$	17	17
24.8^+	$--$	18	$--$
26.9^+	$--$	19	$--$

The variances for treatment 2 are as follow.

$$\widehat{Var}(\widehat{s}(6.9)) = \left(\frac{18}{19}\right)^2 \left[\frac{1}{18(19)}\right] = 0.00262.$$

$$\widehat{Var}(\widehat{s}(7.7)) = \left(\frac{17}{19}\right)^2 \left[\frac{1}{18(19)} + \frac{1}{17(18)}\right] = 0.00496.$$

$$\widehat{Var}(\widehat{s}(8.0)) = \left(\frac{255}{304}\right)^2 \left[\frac{1}{18(19)} + \frac{1}{17(18)} + \frac{1}{15(16)}\right] = 0.00729.$$

$$\widehat{Var}(\widehat{s}(8.3)) = (0.774)^2 \left[\frac{1}{18(19)} + \frac{1}{17(18)} + \frac{1}{15(16)} + \frac{1}{12(13)}\right] = 0.01005.$$

$$\widehat{Var}(\widehat{s}(24.4)) = (0.516)^2 \left[\frac{1}{18(19)} + \frac{1}{17(18)} + \frac{1}{15(16)} + \frac{1}{12(13)} + \frac{1}{2(3)}\right] = 0.04884.$$

The median for treatment 2 cannot be estimated because less than 50% of the observations are uncensored and and the largest observation is censored.

10. Do exercise 4.9 on page 102 of the text book. This is the SAS code and output. There are 5 graphs that accompany this output.

```
data angia_pecgtoris;
input entering lost dying;
cards;
555 0 82
473 8 30
435 8 27
400 7 22
371 7 26
338 28 25
285 31 20
234 32 11
191 24 14
153 27 13
113 22 5
86 23 5
58 18 5
35 9 2
24 7 3
14 11 3
;
run;

data angia_pecgtoris;
retain years -.5;
set angia_pecgtoris;
```

```
freq_ = lost;
years +1;
censored = 0;
output;
freq_ = dying;
censored = 1;
output;
run;

ods graphics on;
ods html ;

proc lifetest data=angia_pecgtoris width = 1  method=life intervals=(0 to 15 by 1)
                  plots=(s,ls,lls,h,p);
time years*censored(0);
freq freq_;
run;

ods off;
ods graphics off;
```

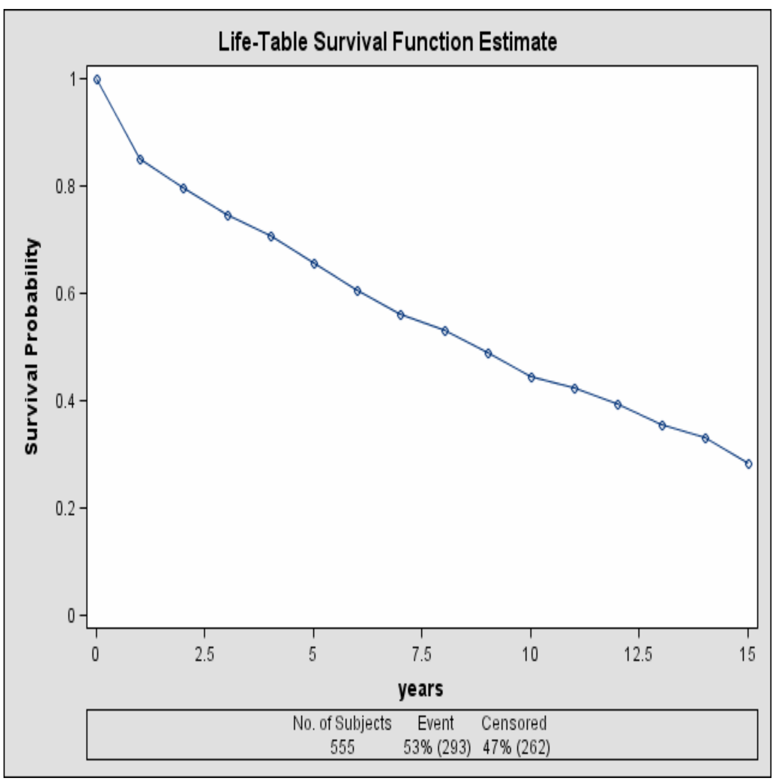

Figure 16.11: This is the survival function graph to Problem 10 (Problem 4.9 in the text book).

```
                                          The SAS System                    17:42 Tuesday, December 30, 2008   3

                                        The LIFETEST Procedure

                                     Life Table Survival Estimates

                                                      Conditional
                                 Effective  Conditional  Probability                      Survival   Median    Median
     Interval        Number   Number     Sample  Probability    Standard                      Standard  Residual  Standard
```

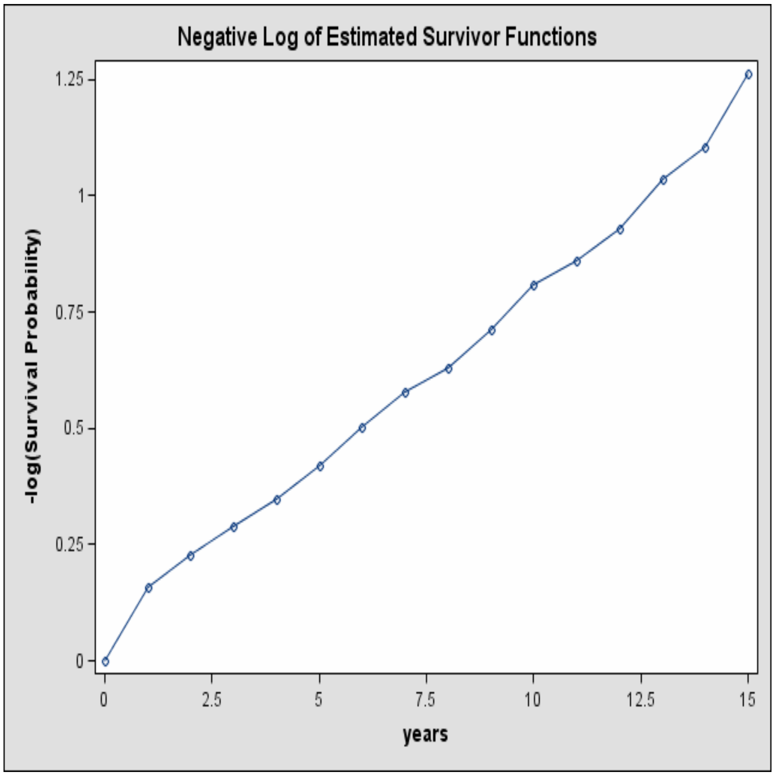

Figure 16.12: This is the negative log of the survival function graph to Problem 10 (Problem 4.9 in the text book).

[Lower,	Upper)	Failed	Censored	Size	of Failure	Error	Survival	Failure	Error	Lifetime	Error
0	1	82	0	555.0	0.1477	0.0151	1.0000	0	0	8.7786	0.5097
1	2	30	8	469.0	0.0640	0.0113	0.8523	0.1477	0.0151	9.8673	0.9019
2	3	27	8	431.0	0.0626	0.0117	0.7977	0.2023	0.0171	9.8577	0.6764
3	4	22	7	396.5	0.0555	0.0115	0.7478	0.2522	0.0185	9.5199	0.4661
4	5	26	7	367.5	0.0707	0.0134	0.7063	0.2937	0.0195	9.0602	0.7924
5	6	25	28	324.0	0.0772	0.0148	0.6563	0.3437	0.0204	9.0647	0.3760
6	7	20	31	269.5	0.0742	0.0160	0.6057	0.3943	0.0212	8.5870	0.3805
7	8	11	32	218.0	0.0505	0.0148	0.5607	0.4393	0.0219	.	.
8	9	14	24	179.0	0.0782	0.0201	0.5324	0.4676	0.0224	.	.
9	10	13	27	139.5	0.0932	0.0246	0.4908	0.5092	0.0232	.	.
10	11	5	22	102.0	0.0490	0.0214	0.4450	0.5550	0.0243	.	.
11	12	5	23	74.5	0.0671	0.0290	0.4232	0.5768	0.0250	.	.
12	13	5	18	49.0	0.1020	0.0432	0.3948	0.6052	0.0263	.	.
13	14	2	9	30.5	0.0656	0.0448	0.3545	0.6455	0.0292	.	.
14	15	3	7	20.5	0.1463	0.0781	0.3313	0.6687	0.0315	.	.
15	.	3	11	8.5	0.3529	0.1639	0.2828	0.7172	0.0373	.	.

Evaluated at the Midpoint of the Interval

Interval [Lower,	Upper)	PDF	PDF Standard Error	Hazard	Hazard Standard Error
0	1	0.1477	0.0151	0.159533	0.017561
1	2	0.0545	0.00968	0.066079	0.012058
2	3	0.0500	0.00937	0.064671	0.012439
3	4	0.0415	0.00866	0.057069	0.012162
4	5	0.0500	0.00955	0.073343	0.014374
5	6	0.0506	0.00986	0.080257	0.016038
6	7	0.0449	0.00980	0.077071	0.017221
7	8	0.0283	0.00839	0.051765	0.015602
8	9	0.0416	0.0108	0.081395	0.021736
9	10	0.0457	0.0123	0.097744	0.027077
10	11	0.0218	0.00959	0.050251	0.022466
11	12	0.0284	0.0124	0.069444	0.031038
12	13	0.0403	0.0173	0.107527	0.048018
13	14	0.0232	0.0160	0.067797	0.047912
14	15	0.0485	0.0263	0.157895	0.090876
15	.	.	.	.	.

Summary of the Number of Censored and Uncensored Values

Total	Failed	Censored	Percent Censored
555	293	262	47.21

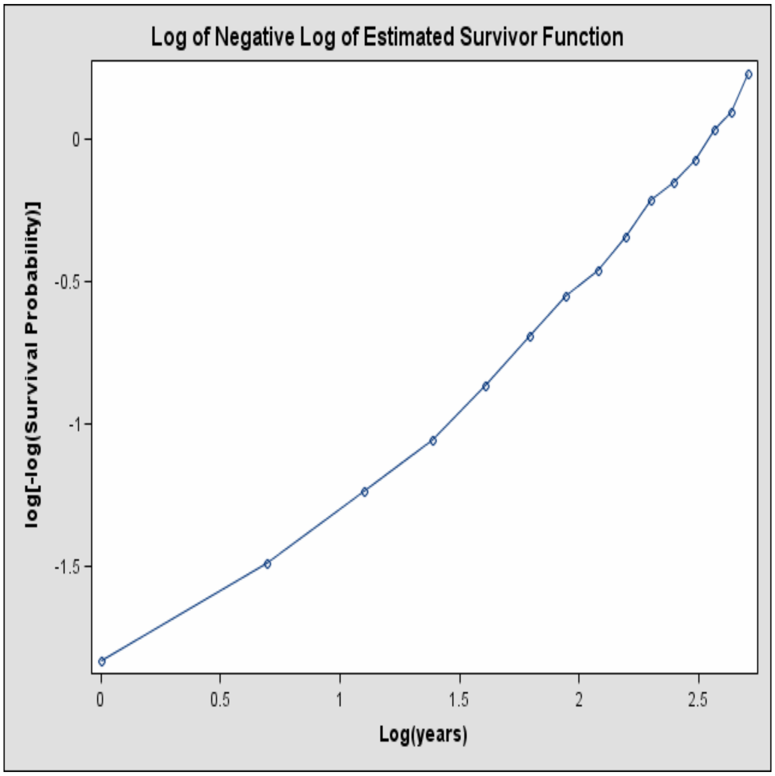

Figure 16.13: This is the log of the negative log of the survival function graph to Problem 10 (Problem 4.9 in the text book).

```
NOTE: There were 1 observations with missing values, negative time values or frequency values less than 1.
```

11. Do exercise 4.6 on page 101 of the text book. The SAS code is as follow.

    This is the Monilia SAS code and the output that goes with Problem 11 (Problem 4.6 in the text book). When the variable `status` equals 0, it indicates the patient has been censored.

```
libname out "d:\statistics\";

data monilia_pos_neg;
input patient survival status posneg $;
cards;
25 24 1 pos
16 38 0 pos
21 51 1 pos
2 64 1 pos
5 66 1 pos
7 70 1 pos
28 72 0 pos
29 91 1 pos
22 117 0 pos
6 180 1 pos
10 191 1 pos
27 8 1 neg
33 29 1 neg
```

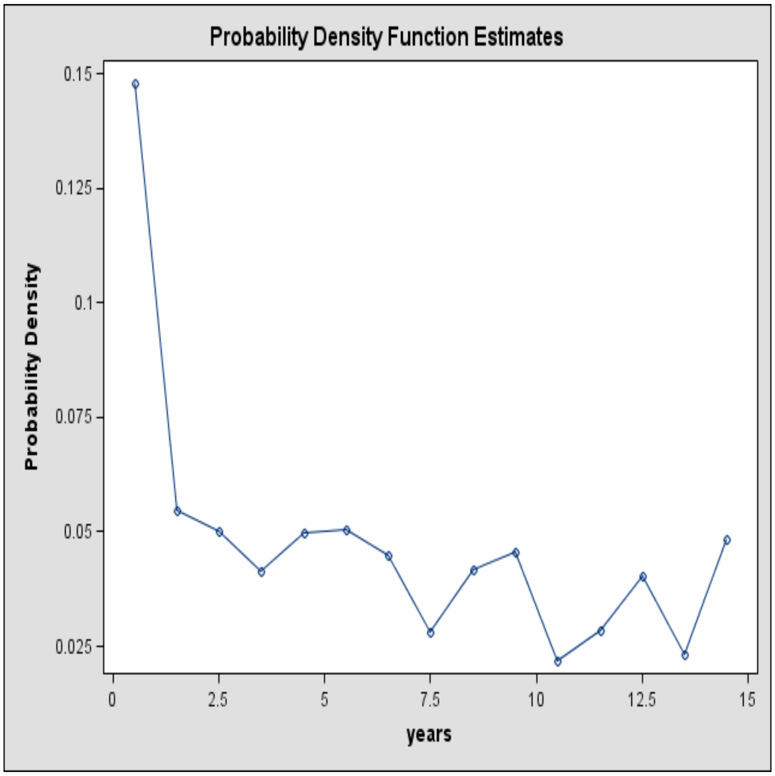

Figure 16.14: This is the pdf function graph to Problem 10 (Problem 4.9 in the text book).

```
30 51 1 neg
26 76 1 neg
32 108 0 neg
23 114 1 neg
24 116 0 neg
13 141 1 neg
14 157 0 neg
20 158 1 neg
15 164 0 neg
17 173 1 neg
9 173 0 neg
1 184 0 neg
31 219 0 neg
3 242 0 neg
11 273 0 neg
18 357 0 neg
4 392 1 neg
12 432 0 neg
8 621 1 neg
19 955 0 neg
;
run;

proc sort data = monilia_pos_neg; by posneg; run;
```

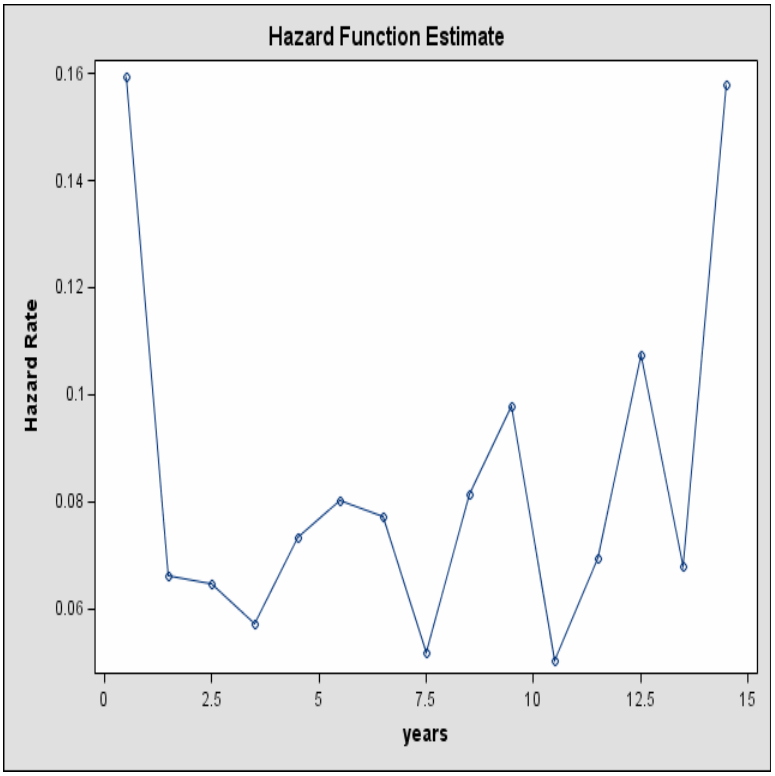

Figure 16.15: This is the hazard function graph to Problem 10 (Problem 4.9 in the text book).

```
ods graphics on;
ods html ;

proc lifetest data = monilia_pos_neg;
time survival*status(0);
strata posneg;
run;


ods off;
ods graphics off;
```

```
                    The SAS System                     15:06 Saturday, December 27, 2008   1

                 The LIFETEST Procedure

                Stratum 1: posneg = neg

            Product-Limit Survival Estimates

                                       Survival
                                       Standard     Number      Number
 survival     Survival    Failure       Error       Failed       Left

   0.000       1.0000          0            0          0          22
   8.000       0.9545     0.0455       0.0444          1          21
  29.000       0.9091     0.0909       0.0613          2          20
  51.000       0.8636     0.1364       0.0732          3          19
  76.000       0.8182     0.1818       0.0822          4          18
 108.000*           .          .            .          4          17
 114.000       0.7701     0.2299       0.0904          5          16
 116.000*           .          .            .          5          15
 141.000       0.7187     0.2813       0.0979          6          14
 157.000*           .          .            .          6          13
 158.000       0.6634     0.3366       0.1048          7          12
 164.000*           .          .            .          7          11
 173.000       0.6031     0.3969       0.1113          8          10
 173.000*           .          .            .          8           9
 184.000*           .          .            .          8           8
 219.000*           .          .            .          8           7
 242.000*           .          .            .          8           6
```

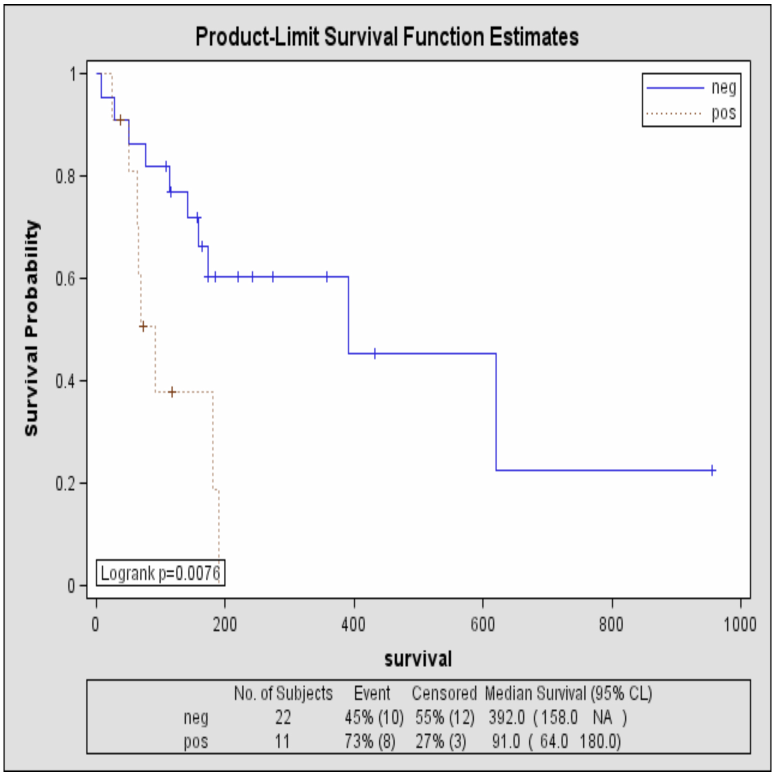

Figure 16.16: This is the Monilia graph to Problem 11 (Problem 4.6 in the text book).

```
273.000*          .          .          .          8          5
357.000*          .          .          .          8          4
392.000      0.4523     0.5477     0.1550          9          3
432.000*          .          .          .          9          2
621.000      0.2262     0.7738     0.1777         10          1
955.000*     0.2262          .          .         10          0

     NOTE: The marked survival times are censored observations.

                      The LIFETEST Procedure

          Summary Statistics for Time Variable survival

                       Quartile Estimates

                         Point     95% Confidence Interval
          Percent      Estimate      [Lower      Upper)

               75       621.000     392.000          .
               50       392.000     158.000          .
               25       141.000      51.000     621.000


                       Mean    Standard Error

                    379.357            62.800

NOTE: The mean survival time and its standard error were underestimated because the largest observation was censored and the
      estimation was restricted to the largest event time.


                         The SAS System                      15:06 Saturday, December 27, 2008   3

                      The LIFETEST Procedure

                     Stratum 2: posneg = pos

                  Product-Limit Survival Estimates

                                           Survival
                                           Standard     Number      Number
 survival     Survival      Failure         Error       Failed       Left

    0.000       1.0000            0             0          0          11
   24.000       0.9091       0.0909        0.0867          1          10
   38.000*           .            .             .          1           9
   51.000       0.8081       0.1919        0.1225          2           8
   64.000       0.7071       0.2929        0.1429          3           7
   66.000       0.6061       0.3939        0.1541          4           6
   70.000       0.5051       0.4949        0.1581          5           5
   72.000*           .            .             .          5           4
   91.000       0.3788       0.6212        0.1613          6           3
```

```
117.000*          .          .          .        6          2
180.000      0.1894     0.8106     0.1563        7          1
191.000           0     1.0000          0        8          0

     NOTE: The marked survival times are censored observations.


           Summary Statistics for Time Variable survival

                         Quartile Estimates

                         Point     95% Confidence Interval
            Percent    Estimate      [Lower      Upper)

                 75     180.000      70.000     191.000
                 50      91.000      64.000     180.000
                 25      64.000      24.000      91.000



                       The LIFETEST Procedure

                         Mean    Standard Error

                      109.290           21.379


     Summary of the Number of Censored and Uncensored Values

                                                          Percent
  Stratum    posneg         Total  Failed    Censored    Censored

        1    neg               22      10          12       54.55
        2    pos               11       8           3       27.27
  ---------------------------------------------------------------
    Total                      33      18          15       45.45


                          The SAS System                    15:06 Saturday, December 27, 2008   5

                       The LIFETEST Procedure

  Testing Homogeneity of Survival Curves for survival over Strata


                          Rank Statistics

                  posneg      Log-Rank    Wilcoxon

                  neg          -4.3706     -90.000
                  pos           4.3706      90.000


            Covariance Matrix for the Log-Rank Statistics

                 posneg           neg          pos

                 neg          2.68375     -2.68375
                 pos         -2.68375      2.68375


            Covariance Matrix for the Wilcoxon Statistics

                 posneg           neg          pos

                 neg          1732.14     -1732.14
                 pos         -1732.14      1732.14


                    Test of Equality over Strata

                                                Pr >
             Test      Chi-Square      DF    Chi-Square

             Log-Rank      7.1178       1      0.0076
             Wilcoxon      4.6763       1      0.0306
             -2Log(LR)     8.2430       1      0.0041
```

This is the SAS code and output for mumps.

```
data mumps;
input patient survival status posneg $;
cards;
25 24 1 pos
16 38 0 pos
21 51 1 pos
2 64 1 pos
7 70 1 pos
28 72 0 pos
32 108 0 pos
23 114 1 pos
24 116 0 pos
```

```
22 117 0 pos
15 164 0 pos
6 180 1 pos
1 184 0 pos
10 191 1 pos
31 219 0 pos
3 242 0 pos
11 273 0 pos
18 357 0 pos
12 432 0 pos
27 8 1 neg
33 29 1 neg
26 76 1 neg
29 91 1 neg
13 141 1 neg
14 157 0 neg
17 173 1 neg
9 173 0 neg
4 392 1 neg
19 955 0 neg
;
run;

proc sort data = mumps; by posneg; run;


ods graphics on;
ods html ;

proc lifetest data = mumps;
time survival*status(0);
strata posneg;
run;


ods off;
ods graphics off;
```

```
                          The SAS System                    16:05 Saturday, December 27, 2008   1

                        The LIFETEST Procedure

                       Stratum 1: posneg = neg

                   Product-Limit Survival Estimates

                                             Survival
                                             Standard     Number      Number
     survival     Survival      Failure        Error      Failed        Left

       0.000       1.0000            0            0          0          10
       8.000       0.9000       0.1000       0.0949          1           9
      29.000       0.8000       0.2000       0.1265          2           8
      76.000       0.7000       0.3000       0.1449          3           7
      91.000       0.6000       0.4000       0.1549          4           6
     141.000       0.5000       0.5000       0.1581          5           5
     157.000*           .            .            .          5           4
     173.000       0.3750       0.6250       0.1606          6           3
     173.000*           .            .            .          6           2
     392.000       0.1875       0.8125       0.1550          7           1
     955.000*      0.1875            .            .          7           0

           NOTE: The marked survival times are censored observations.


                 Summary Statistics for Time Variable survival
```

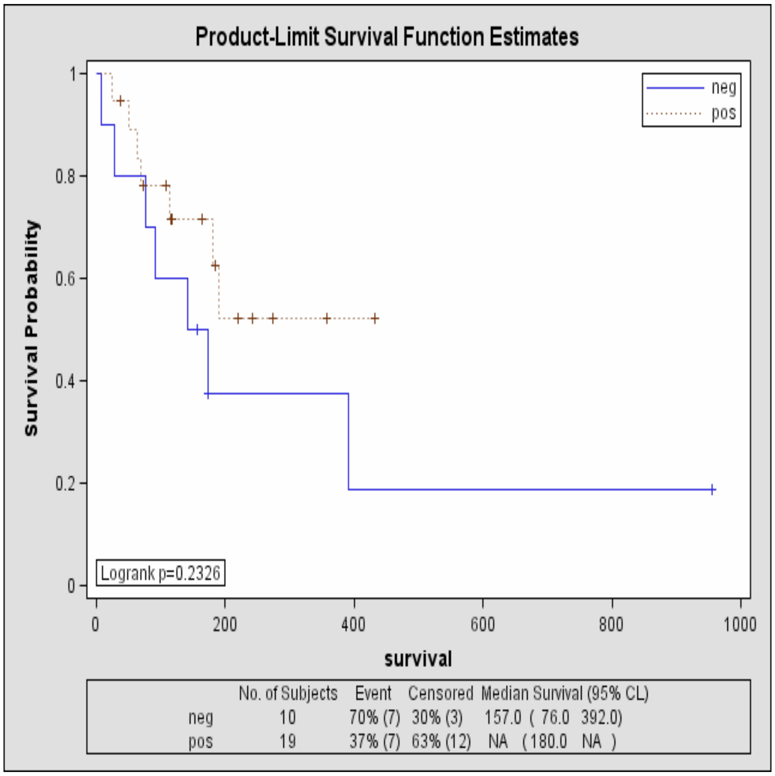

Figure 16.17: This is the Mumps graph to Problem 11 (Problem 4.6 in the text book).

Quartile Estimates

Percent	Point Estimate	95% Confidence Interval [Lower	Upper)
75	392.000	141.000	.
50	157.000	76.000	392.000
25	76.000	8.000	173.000

Mean	Standard Error
203.125	53.696

Product-Limit Survival Estimates

survival	Survival	Failure	Survival Standard Error	Number Failed	Number Left
0.000	1.0000	0	0	0	19
24.000	0.9474	0.0526	0.0512	1	18
38.000*	.	.	.	1	17
51.000	0.8916	0.1084	0.0724	2	16
64.000	0.8359	0.1641	0.0867	3	15
70.000	0.7802	0.2198	0.0972	4	14
72.000*	.	.	.	4	13
108.000*	.	.	.	4	12
114.000	0.7152	0.2848	0.1087	5	11
116.000*	.	.	.	5	10
117.000*	.	.	.	5	9
164.000*	.	.	.	5	8
180.000	0.6258	0.3742	0.1267	6	7
184.000*	.	.	.	6	6
191.000	0.5215	0.4785	0.1421	7	5
219.000*	.	.	.	7	4
242.000*	.	.	.	7	3
273.000*	.	.	.	7	2
357.000*	.	.	.	7	1
432.000*	0.5215	.	.	7	0

NOTE: The marked survival times are censored observations.

Percent	Point Estimate	95% Confidence Interval [Lower	Upper)
75	.	191.000	.
50	.	180.000	.
25	114.000	51.000	.

```
                    Mean    Standard Error

                 154.599           14.771

NOTE: The mean survival time and its standard error were underestimated because the largest observation was censored and the
      estimation was restricted to the largest event time.

              Summary of the Number of Censored and Uncensored Values

                                                          Percent
        Stratum    posneg        Total  Failed    Censored    Censored

              1    neg              10       7           3       30.00
              2    pos              19       7          12       63.16
        ---------------------------------------------------------------
          Total                     29      14          15       51.72

                          The SAS System                    16:05 Saturday, December 27, 2008   5

                       The LIFETEST Procedure

        Testing Homogeneity of Survival Curves for survival over Strata


                           Rank Statistics

                    posneg      Log-Rank    Wilcoxon

                    neg           2.0850      38.000
                    pos          -2.0850     -38.000


              Covariance Matrix for the Log-Rank Statistics

                   posneg           neg           pos

                   neg          3.05042      -3.05042
                   pos         -3.05042       3.05042


              Covariance Matrix for the Wilcoxon Statistics

                   posneg           neg           pos

                   neg          1290.00      -1290.00
                   pos         -1290.00       1290.00


                     Test of Equality over Strata

                                                Pr >
                Test      Chi-Square      DF    Chi-Square

                Log-Rank      1.4251       1      0.2326
                Wilcoxon      1.1194       1      0.2901
                -2Log(LR)     0.3519       1      0.5530
```

The SAS code and output for PPD is as follow.

```
data PPD;
input patient survival status posneg $;
cards;
27 8 1 neg
25 24 1 neg
33 29 1 neg
16 38 0 neg
30 51 1 neg
21 51 1 neg
2 64 1 neg
7 70 1 neg
26 76 1 neg
29 91 1 neg
32 108 0 neg
24 116 0 neg
22 117 0 neg
13 141 1 neg
15 164 0 neg
17 173 1 neg
9 173 0 neg
6 180 1 neg
```

```
1 184 0 neg
31 219 0 neg
3 242 0 neg
18 357 0 neg
4 392 1 neg
12 432 0 neg
8 621 1 neg
19 955 0 neg
5 66 1 pos
28 72 0 pos
23 114 1 pos
14 157 0 pos
10 191 1 pos
11 273 0 pos
;
run;

proc sort data = PPD; by posneg; run;


ods graphics on;
ods html ;

proc lifetest data = PPD method = pl;
time survival*status(0);
strata posneg;
run;


ods off;
ods graphics off;
```

```
                         The SAS System                    16:54 Saturday, December 27, 2008   1

                      The LIFETEST Procedure

                     Stratum 1: posneg = neg

                 Product-Limit Survival Estimates

                                              Survival
                                              Standard      Number       Number
        survival      Survival     Failure     Error        Failed        Left

           0.000       1.0000           0           0         0            26
           8.000       0.9615      0.0385      0.0377         1            25
          24.000       0.9231      0.0769      0.0523         2            24
          29.000       0.8846      0.1154      0.0627         3            23
          38.000*           .           .           .         3            22
          51.000            .           .           .         4            21
          51.000       0.8042      0.1958      0.0786         5            20
          64.000       0.7640      0.2360      0.0844         6            19
          70.000       0.7238      0.2762      0.0890         7            18
          76.000       0.6836      0.3164      0.0927         8            17
          91.000       0.6434      0.3566      0.0956         9            16
         108.000*           .           .           .         9            15
         116.000*           .           .           .         9            14
         117.000*           .           .           .         9            13
         141.000       0.5939      0.4061      0.1002        10            12
         164.000*           .           .           .        10            11
         173.000       0.5399      0.4601      0.1046        11            10
         173.000*           .           .           .        11             9
         180.000       0.4799      0.5201      0.1089        12             8
         184.000*           .           .           .        12             7
         219.000*           .           .           .        12             6
         242.000*           .           .           .        12             5
         357.000*           .           .           .        12             4
         392.000       0.3599      0.6401      0.1321        13             3
         432.000*           .           .           .        13             2
         621.000       0.1800      0.8200      0.1434        14             1
         955.000*      0.1800           .           .        14             0

              NOTE: The marked survival times are censored observations.


                  Summary Statistics for Time Variable survival
```

```
                             Quartile Estimates

                              Point     95% Confidence Interval
                 Percent    Estimate      [Lower      Upper)

                      75     621.000     392.000        .
                      50     180.000      91.000     621.000
                      25      70.000      51.000     173.000


                              Mean    Standard Error

                           316.206           58.499

NOTE: The mean survival time and its standard error were underestimated because the largest observation was censored and the
                     estimation was restricted to the largest event time.


                           The LIFETEST Procedure

                          Stratum 2: posneg = pos

                      Product-Limit Survival Estimates

                                               Survival
                                               Standard     Number      Number
        survival     Survival    Failure        Error       Failed       Left

          0.000       1.0000          0            0          0           6
         66.000       0.8333     0.1667       0.1521          1           5
         72.000*           .          .            .          1           4
        114.000       0.6250     0.3750       0.2135          2           3
        157.000*           .          .            .          2           2
        191.000       0.3125     0.6875       0.2454          3           1
        273.000*      0.3125          .            .          3           0

            NOTE: The marked survival times are censored observations.


                 Summary Statistics for Time Variable survival

                             Quartile Estimates

                              Point     95% Confidence Interval
                 Percent    Estimate      [Lower      Upper)

                      75        .        114.000        .
                      50     191.000     114.000        .
                      25     114.000      66.000        .


                              Mean    Standard Error

                           154.125           26.035

NOTE: The mean survival time and its standard error were underestimated because the largest observation was censored and the
                     estimation was restricted to the largest event time.


                           The LIFETEST Procedure

               Summary of the Number of Censored and Uncensored Values

                                                                  Percent
           Stratum    posneg         Total  Failed    Censored    Censored

                1     neg               26      14          12       46.15
                2     pos                6       3           3       50.00
          -------------------------------------------------------------------
             Total                      32      17          15       46.88
                               The SAS System                      16:54 Saturday, December 27, 2008   5

                           The LIFETEST Procedure

          Testing Homogeneity of Survival Curves for survival over Strata


                              Rank Statistics

                        posneg      Log-Rank    Wilcoxon

                        neg          0.01693      15.000
                        pos         -0.01693     -15.000


                 Covariance Matrix for the Log-Rank Statistics

                      posneg           neg           pos

                      neg          2.39082      -2.39082
                      pos         -2.39082       2.39082


                 Covariance Matrix for the Wilcoxon Statistics

                      posneg           neg           pos

                      neg          1326.22      -1326.22
                      pos         -1326.22       1326.22


                       Test of Equality over Strata

                                                    Pr >
```

Test	Chi-Square	DF	Chi-Square
Log-Rank	0.0001	1	0.9913
Wilcoxon	0.1697	1	0.6804
-2Log(LR)	0.1139	1	0.7358

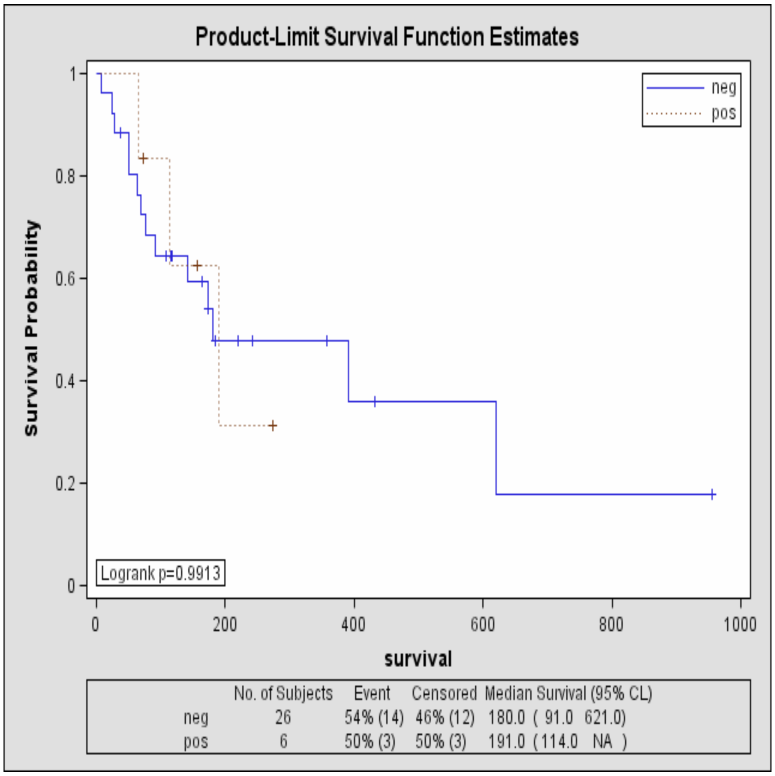

Figure 16.18: This is the PPD graph to Problem 11 (Problem 4.6 in the text book).

This is the output for PHA. The SAS code is very similar to the previous code and has been omitted.

```
                         The SAS System                     12:24 Sunday, December 28, 2008   1

                       The LIFETEST Procedure

                      Stratum 1: posneg = neg

                  Product-Limit Survival Estimates

                                                 Survival
                                                 Standard     Number      Number
      survival     Survival     Failure          Error       Failed        Left

         0.000      1.0000            0              0            0          11
        51.000      0.9091       0.0909         0.0867            1          10
        66.000      0.8182       0.1818         0.1163            2           9
        70.000      0.7273       0.2727         0.1343            3           8
       116.000*          .            .              .            3           7
       141.000      0.6234       0.3766         0.1500            4           6
       158.000      0.5195       0.4805         0.1569            5           5
       173.000      0.4156       0.5844         0.1562            6           4
       173.000*          .            .              .            6           3
       180.000      0.2771       0.7229         0.1537            7           2
       392.000      0.1385       0.8615         0.1245            8           1
       955.000*     0.1385            .              .            8           0

       NOTE: The marked survival times are censored observations.


             Summary Statistics for Time Variable survival

                          Quartile Estimates

                           Point      95% Confidence Interval
              Percent     Estimate       [Lower       Upper)

                   75      392.000      158.000           .
                   50      173.000       70.000     392.000
                   25       70.000       51.000     173.000
```

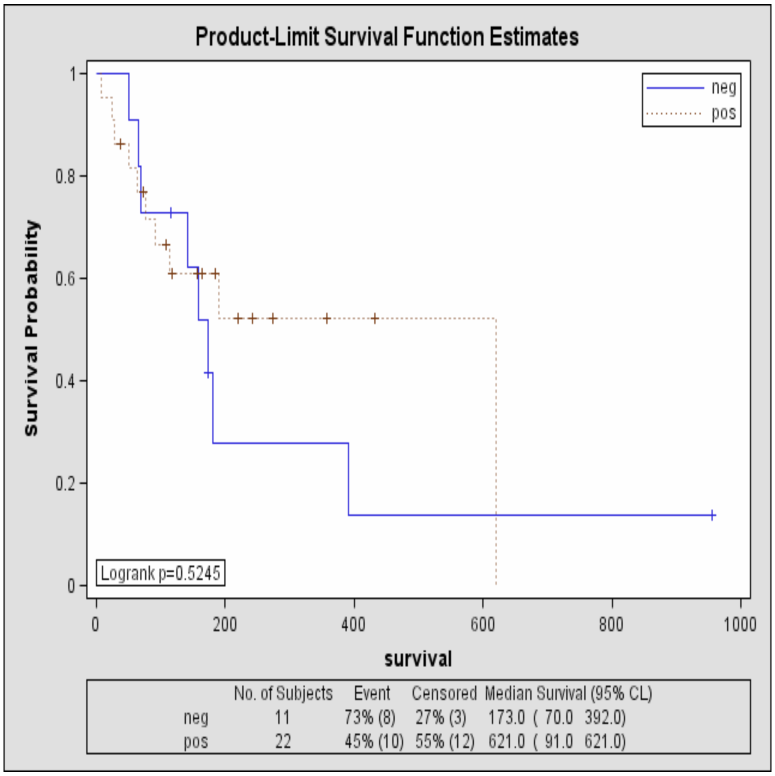

Figure 16.19: This is the PHA graph to Problem 11 (Problem 4.6 in the text book).

The LIFETEST Procedure

Mean	Standard Error
199.580	44.363

NOTE: The mean survival time and its standard error were underestimated because the largest observation was censored and the estimation was restricted to the largest event time.

Stratum 2: posneg = pos

Product-Limit Survival Estimates

survival	Survival	Failure	Survival Standard Error	Number Failed	Number Left
0.000	1.0000	0	0	0	22
8.000	0.9545	0.0455	0.0444	1	21
24.000	0.9091	0.0909	0.0613	2	20
29.000	0.8636	0.1364	0.0732	3	19
38.000*	.	.	.	3	18
51.000	0.8157	0.1843	0.0834	4	17
64.000	0.7677	0.2323	0.0912	5	16
72.000*	.	.	.	5	15
76.000	0.7165	0.2835	0.0985	6	14
91.000	0.6653	0.3347	0.1039	7	13
108.000*	.	.	.	7	12
114.000	0.6099	0.3901	0.1090	8	11
117.000*	.	.	.	8	10
157.000*	.	.	.	8	9
164.000*	.	.	.	8	8
184.000*	.	.	.	8	7
191.000	0.5228	0.4772	0.1234	9	6
219.000*	.	.	.	9	5
242.000*	.	.	.	9	4
273.000*	.	.	.	9	3
357.000*	.	.	.	9	2
432.000*	.	.	.	9	1
621.000	0	1.0000	0	10	0

NOTE: The marked survival times are censored observations.

The LIFETEST Procedure

Summary Statistics for Time Variable survival

Quartile Estimates

```
                   Point     95% Confidence Interval
        Percent    Estimate      [Lower      Upper)

             75     621.000        .           .
             50     621.000      91.000     621.000
             25      76.000      29.000     621.000


                   Mean    Standard Error

                364.427           68.019


   Summary of the Number of Censored and Uncensored Values

                                                         Percent
Stratum    posneg         Total  Failed    Censored    Censored

      1    neg               11       8           3       27.27
      2    pos               22      10          12       54.55
---------------------------------------------------------------
  Total                      33      18          15       45.45

                     The SAS System                       12:24 Sunday, December 28, 2008   5

                 The LIFETEST Procedure

Testing Homogeneity of Survival Curves for survival over Strata


                    Rank Statistics

          posneg       Log-Rank    Wilcoxon

          neg            1.2917      6.0000
          pos           -1.2917     -6.0000


       Covariance Matrix for the Log-Rank Statistics

         posneg           neg           pos

         neg          4.11941      -4.11941
         pos         -4.11941       4.11941


       Covariance Matrix for the Wilcoxon Statistics

         posneg           neg           pos

         neg          2083.86      -2083.86
         pos         -2083.86       2083.86


              Test of Equality over Strata

                                         Pr >
        Test       Chi-Square     DF    Chi-Square

        Log-Rank      0.4050       1      0.5245
        Wilcoxon      0.0173       1      0.8954
        -2Log(LR)     0.1136       1      0.7361
```

The SAS output for SK-SD follows. The SAS code has been omitted. It is similar to the code above.

```
                     The SAS System                       12:46 Sunday, December 28, 2008   1

                 The LIFETEST Procedure

                Stratum 1: posneg = neg

              Product-Limit Survival Estimates

                                          Survival
                                          Standard      Number      Number
  survival     Survival    Failure         Error        Failed        Left

    0.000       1.0000           0             0          0            29
    8.000       0.9655      0.0345        0.0339          1            28
   24.000       0.9310      0.0690        0.0471          2            27
   29.000       0.8966      0.1034        0.0566          3            26
   38.000*           .           .             .          3            25
   51.000            .           .             .          4            24
   51.000       0.8248      0.1752        0.0712          5            23
   64.000       0.7890      0.2110        0.0766          6            22
   66.000       0.7531      0.2469        0.0811          7            21
   72.000*           .           .             .          7            20
   76.000       0.7154      0.2846        0.0853          8            19
   91.000       0.6778      0.3222        0.0888          9            18
  108.000*           .           .             .          9            17
  114.000       0.6379      0.3621        0.0921         10            16
  116.000*           .           .             .         10            15
  117.000*           .           .             .         10            14
  141.000       0.5924      0.4076        0.0961         11            13
  157.000*           .           .             .         11            12
  158.000       0.5430      0.4570        0.1000         12            11
  173.000       0.4936      0.5064        0.1024         13            10
  173.000*           .           .             .         13             9
  180.000       0.4388      0.5612        0.1046         14             8
  184.000*           .           .             .         14             7
  191.000       0.3761      0.6239        0.1068         15             6
  219.000*           .           .             .         15             5
```

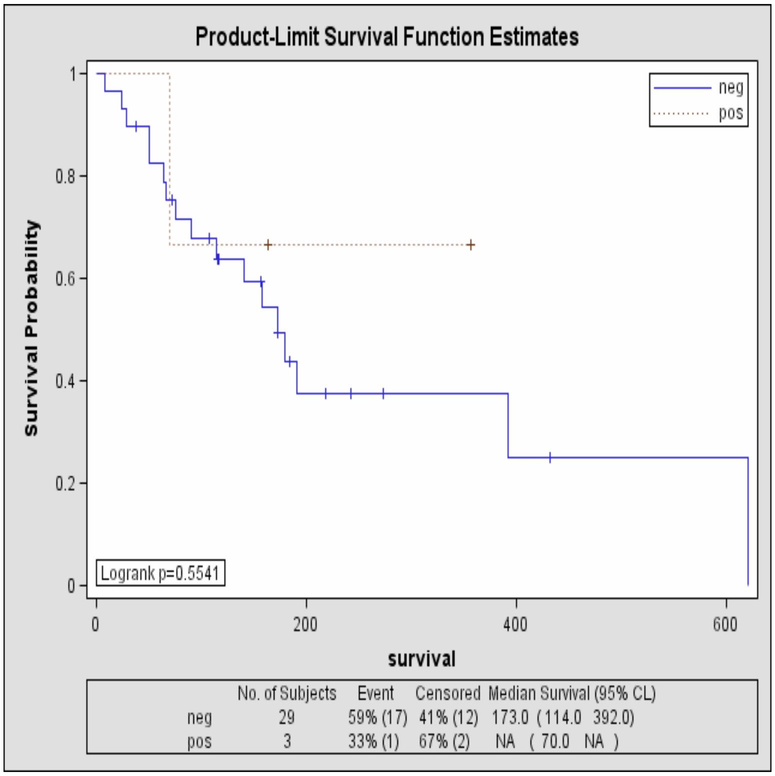

Figure 16.20: This is the SK-SD graph to Problem 11 (Problem 4.6 in the text book).

```
  242.000*           .           .           .        15           4
  273.000*           .           .           .        15           3
  392.000       0.2507      0.7493      0.1247        16           2
  432.000*           .           .           .        16           1
  621.000            0      1.0000           0        17           0

                      The LIFETEST Procedure

     NOTE: The marked survival times are censored observations.


           Summary Statistics for Time Variable survival

                          Quartile Estimates

                          Point     95% Confidence Interval
            Percent    Estimate      [Lower       Upper)

                 75     621.000     180.000     621.000
                 50     173.000     114.000     392.000
                 25      76.000      51.000     158.000


                          Mean    Standard Error

                       270.715            53.203

                      Stratum 2: posneg = pos

                   Product-Limit Survival Estimates

                                           Survival
                                           Standard     Number      Number
 survival      Survival     Failure         Error       Failed       Left

    0.000        1.0000           0            0           0           3
   70.000        0.6667      0.3333       0.2722           1           2
  164.000*            .           .            .           1           1
  357.000*       0.6667           .            .           1           0

     NOTE: The marked survival times are censored observations.


           Summary Statistics for Time Variable survival

                          Quartile Estimates

                          Point     95% Confidence Interval
            Percent    Estimate      [Lower       Upper)

                 75          .       70.000           .
                 50          .       70.000           .
```

```
                    25      70.000      70.000        .

                              Mean    Standard Error

                            70.000             .

NOTE: The mean survival time and its standard error were underestimated because the largest observation was censored and the
                                     estimation was restricted to the largest event time.


                            The LIFETEST Procedure

              Summary of the Number of Censored and Uncensored Values

                                                              Percent
           Stratum    posneg         Total  Failed    Censored    Censored

                 1    neg               29      17          12       41.38
                 2    pos                3       1           2       66.67
           -------------------------------------------------------------
             Total                      32      18          14       43.75

                                The SAS System                       12:46 Sunday, December 28, 2008   5

                            The LIFETEST Procedure

           Testing Homogeneity of Survival Curves for survival over Strata


                               Rank Statistics

                       posneg      Log-Rank    Wilcoxon

                       neg          0.73280      13.000
                       pos         -0.73280     -13.000


                  Covariance Matrix for the Log-Rank Statistics

                      posneg           neg           pos

                      neg          1.53424      -1.53424
                      pos         -1.53424       1.53424


                  Covariance Matrix for the Wilcoxon Statistics

                      posneg           neg           pos

                      neg          785.444      -785.444
                      pos         -785.444       785.444


                         Test of Equality over Strata

                                                    Pr >
                 Test      Chi-Square      DF    Chi-Square

                 Log-Rank      0.3500       1      0.5541
                 Wilcoxon      0.2152       1      0.6427
                 -2Log(LR)     0.7492       1      0.3867
```

Summary: The median survival time of someone who tests positive for Monilia is about 70 days as opposed to approximately 392 days for someone who tests negative. The skin test for Monilia might be a good predictor of survival time. For someone who tests negative for mumps, the median survival time is 141 days and the median survival time for someone who tests positive is greater than 191 days. This is inconclusive. The median survival time of someone who test postive for PPD is $114 < m < 191$ and $173 < m < 180$ for someone who tests negative. This is inconclusive. The median survival time of someone who tests positive for PHA is $191 < m < 621$ and $158 < m < 173$ for someone who test negative. This might be a good predictor of survival time. The median survival time of someone who tests negative for SK-SD is approximately 173 days and more than 70 days for someone who tests positive. This is inconclusive.

12. Prove that $\prod_{j=1}^{k+1}(p_1p_2\cdots p_{j-1}q_j)^{d_j} = \prod_j q_j^{d_j} p_j^{n_j-d_j}$.

16.10 Midterm Exam and Answers

Do any five problems.

1. Let the hazard function $h(t)$ be given by $h(t) = \theta_0 + \theta_1 t^{\theta_2}$, $t > 0$, $\theta_0 > 0$, $\theta_2 > 0$. Derive the density function corresponding to this $h(t)$. Solution: $h(t) = \theta_0 + \theta_1 r^{\theta_2} = \frac{f(t)}{s(t)}$. We know that $\log s(t) = H(t)$, $s(t) = e^{-H(t)}$. Find $H(t)$.

$$\int_0^t h(x), dx = \int_0^t \theta_0 + \theta_1 x^{\theta_2}\, dx = \theta_0 x + \frac{\theta_1 x^{\theta_2+1}}{\theta_2+1}\Big|_0^t = \theta_0 t + \frac{\theta_1 t^{\theta_2+1}}{\theta_2+1} \Rightarrow$$

$$s(t) = e^{-\left[\theta_0 t + \frac{\theta_1 t^{\theta_2+1}}{\theta_2+1}\right]} \Rightarrow f(t) = h(t)s(t) = \left[\theta_0 + \theta_1 t^{\theta_2}\right] e^{-\left[\theta_0 t + \frac{\theta_1 t^{\theta_2+1}}{\theta_2+1}\right]}.$$

2. Consider the density function of the logistic distribution given by $f(y) = e^{y-\mu)/\sigma} \Big/ \left[\sigma\{1+e^{(y-\mu)/\sigma}\}^2\right]$., $-\infty < y < \infty$. Derive the survival function of $T = e^y$. Solution: $y = \log T$. $\frac{dy}{dT} = \frac{1}{T}$.

$$f(T) = \frac{e^{[\log T-\mu]/\sigma}}{T\sigma\{1+e^{[\log T-\mu]/\sigma}\}^2}, 0 < T < \infty.$$

$$S(T) = 1 - F(T).$$

Find $F(T)$:

$$\int_0^t \frac{e^{[\log x-\mu]/\sigma}}{x\sigma\{1+e^{[\log x-\mu]/\sigma}\}^2}\, dx$$

Finish the integration.

3. Let $X_{(r)}$ be the r^{th} order statistic in a sample of size n from $\exp(\theta)$. Derive $E(X_{(r)})$. Solution: Let $x_1, x_2, ..., x_n$ be a random sample.

$$f(\underline{x}|\theta) = \frac{n!}{\theta^2} e^{-\frac{\sum x_i}{\theta}},$$

$u_1 = x_1$, $u_i = x_i - x_{i-1}$, $i = 2, 3, ..., n$. $x_i = \sum_{j=1}^{i} u_i, i = 1, 2, ..., n$. $|J| = 1$. Then,

$$f(\underline{x}|\theta)\, d\underline{x} = \frac{n!}{\theta^n} e^{\sum_i \sum_{j=1}^{i} \frac{u_i}{\theta}}\, du_1\, du_2 \cdots du_n = \prod_{i=1}^{n} \left(\frac{n-i+1}{\theta} e^{\frac{-u_i(n-i+1)}{\theta}}\, d\,u_i\right) \Rightarrow u_i \sim \exp\left(\frac{\theta}{n-i+1}\right).$$

$E(u_i) = \frac{\theta}{n-i+1}$. $E(x_{(r)}) = E\left(\sum_{i=1}^{r} u_i\right) = \sum_{i=1}^{r} \frac{\theta}{n-i+1}$.

4. Consider the remission time of 21 lukemia patients: $6, 6, 6, 7, 10, 13, 16, 22, 23, 6^+, 9^+, 10^+, 11^+, 17^+, 19^+, 20^+, 25^+, 32^+, 32^+, 34^+, 35^+$. Compute the PL estimator of $s(t)$ and plot this estimator. The SAS code to solve this problem is as follow. When the variable `STATUS` equals to 0, it means that the observation is censored.

```
data test;
input y status;
cards;
6 1
6 1
6 1
6 0
7 1
9 0
```

```
10 1
10 0
11 0
13 1
16 1
17 0
19 0
20 0
22 1
23 1
25 0
32 0
32 0
34 0
35 0
;
run;

ods html;
ods graphics on;


proc lifetest data = test;
time y*status(0);
run;

ods graphics off;
ods off;
```

```
                              The SAS System                    13:48 Thursday, December 25, 2008   1

                            The LIFETEST Procedure

                        Product-Limit Survival Estimates

                                            Survival
                                            Standard     Number      Number
            y      Survival    Failure       Error       Failed       Left

       0.0000       1.0000           0           0          0          21
       6.0000            .           .           .          1          20
       6.0000            .           .           .          2          19
       6.0000       0.8571      0.1429      0.0764          3          18
       6.0000*           .           .           .          3          17
       7.0000       0.8067      0.1933      0.0869          4          16
       9.0000*           .           .           .          4          15
      10.0000       0.7529      0.2471      0.0963          5          14
      10.0000*           .           .           .          5          13
      11.0000*           .           .           .          5          12
      13.0000       0.6902      0.3098      0.1068          6          11
      16.0000       0.6275      0.3725      0.1141          7          10
      17.0000*           .           .           .          7           9
      19.0000*           .           .           .          7           8
      20.0000*           .           .           .          7           7
      22.0000       0.5378      0.4622      0.1282          8           6
      23.0000       0.4482      0.5518      0.1346          9           5
      25.0000*           .           .           .          9           4
      32.0000*           .           .           .          9           3
      32.0000*           .           .           .          9           2
      34.0000*           .           .           .          9           1
      35.0000*      0.4482           .           .          9           0

                              Point      95% Confidence Interval
                  Percent    Estimate      [Lower      Upper)

                     75          .         23.0000        .
                     50      23.0000       13.0000        .
                     25      13.0000        6.0000     23.0000


                              Mean    Standard Error

                           17.9092          1.6474

NOTE: The mean survival time and its standard error were underestimated because the largest observation was censored and the
      estimation was restricted to the largest event time.


                  Summary of the Number of Censored and Uncensored Values
```

Total	Failed	Censored	Percent Censored
21	9	12	57.14

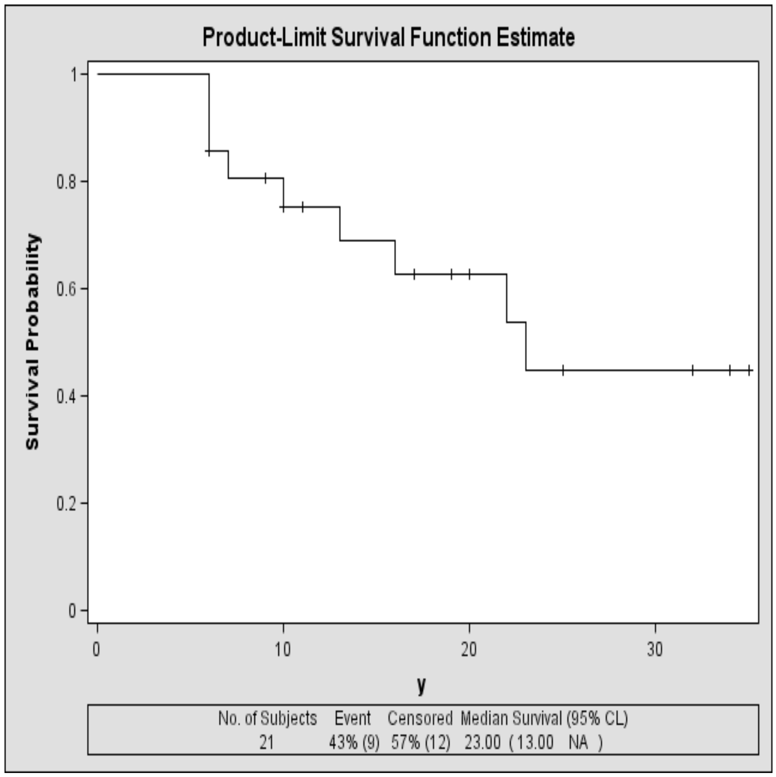

Figure 16.21: This is the graph to Problem 4 of the Mid-Term Exam.

5. Consider the data given in Problem 4. Check graphically if $\exp(\theta)$ is a good fit to this data. Give $\widehat{\theta}$ for this data which is the mle of θ.

6. Prove that IFR $\Rightarrow$ IFRA. See page 1119 of these notes for the solution.

16.11 Plotting $F(x)$ and $F_n(x)$

Normal and Exponential Distribution

Here $F_n(x)$ is the empirical distribution function or the product limit estimator of $F(x)$. Assume some form for $F(x)$. For example, the exponential distribution, $F(x) = 1-e^{-\lambda x}$. Normal probability paper transforms a plot of $(t, F(t))$ to a straight line. Consider the exponential function $\exp(\lambda)$. $F(t) = 1-e^{-\lambda t}$. $e^{-\lambda t} = 1-F(t)$. $-\lambda t = \log(1-F(t))$. $t = -\frac{1}{\lambda}\log(1-F(t)) = g(t)$. A graph paper that transforms $F(t)$ to $g(t)$ is going to give a straight line fit if we plot $(t, F_n(t))$. We need to estimate λ. Consider the example on pages 164-165 of the text book. $\Pi_{0.632} = \frac{1}{\lambda} \Rightarrow \widehat{\lambda} = \frac{1}{\widehat{\Pi}_{0.632}}$.

Weibull Distribution

Consider the Weibull distribution. $F(t) = 1 - e^{-(\lambda t)^{\delta}}$. $\log t = -\log\lambda + \frac{1}{\delta}\log(\log(1-F(t)^{-1}) = g(t)$. Graph paper transforms t to $\log t$ and F to $g(t)$.

Example: Consider the example on page 166 of the text book. Since the graph shows a linear fit, the function is a good fit.

We can estimate λ and δ from percentiles.

$$\int_0^{\pi_p} \lambda e^{-\lambda u}\, du = p,$$

$$\left.\frac{\lambda e^{-\lambda u}}{-\lambda}\right|_{-}^{\pi_p} = p,$$

$$1 - e^{-\lambda \pi_p} = p$$

$$1 - p = e^{-\lambda \pi_p} \Rightarrow \lambda = -\frac{1}{\pi_p}\log(1-p).$$

This finds p such that $\pi_p = \frac{1}{\lambda}$ for the exponent.

Log-Normal Distribution

If $\log T \sim N(\mu, \sigma^2)$, then $T \sim \log -Normal(\mu, \sigma^2)$. $F(T) = P(T \le t) = P(\log T \le \log t) = P\left(\frac{\log T - \mu}{\sigma} \le \frac{\log t - \mu}{\sigma}\right) = P\left(Z \le \frac{\log t - \mu}{\sigma}\right) = \Phi\left(\frac{\log t - \mu}{\sigma}\right)$. Then, $\left(\frac{\log t - \mu}{\sigma}\right) = \Phi^{-1}(f(t))$. $logt = \mu + \sigma \Phi^{-1} F(t) = g(t)$.

Example: Consider the example on pages 168-169 of the text book. The survival time of 20 insects exposed to insecticide. The plot on page 169 should be a straight line.

Gamma Distribution

The incomplete gamma distribution is $I_\delta(t) = \int_0^t e^{-u} u^{\delta-1}\, du$.

$$F(t) = \lambda^u \int_0^t \frac{e^{-\lambda u} u^{\delta-1}}{\Gamma(\delta)}\, du = \frac{1}{\Gamma(\delta)} I_\delta(\lambda t).$$

$t = \frac{1}{\lambda} I_\delta^{-1}[\Gamma(\delta)F(t)] = g(t)$ because $I_\delta(\lambda t) = \Gamma(\delta)F(t)$, $\lambda t = I_\delta^{-1}[\Gamma(\delta)F(t)]$. Another way of getting linear plots is to plot $[x(p), y(p)]$ where $x(p) = 100p^{th}$ sample percentile and $y(p) = 100p^{th}$ estimate population percentile. Let $t_1 < t_2 < \cdots < t_n$ be the data. $b_i = \frac{i-0.5}{n}$, $i = 1, 2, ..., n$ or use $b_i = \frac{i}{n+1}$. $F_n(t_i) = \frac{i-0.5}{n} = b_i$. $t_1, t_2, ..., t_n$ are sample percentiles corresponding to probabilities $b_1, b_2, ..., b_n$. How do we get the population percentiles? Let $F(t|\theta)$ be the cdf. Then, for the population percentile t_i^*, solve $F(t_i^*|\widehat{\theta}) = b_i$. Then, plot (t_i, t_i^*). We would like to have a straight $45°$ line. For the gamma distribution,

$$F(t) = \frac{1}{\Gamma(\delta)} \int_0^{\lambda t} e^{-u} u^{\lambda-1}\, du.$$

$$F(t_i^*|\widehat{\theta}) = \frac{1}{\Gamma(\widehat{\delta})} \int_0^{\widehat{\lambda} t_i^*} e^{-u} u^{\widehat{\lambda}-1}\, du = b_i$$

and solve for t_i^*. See the example on pages 172-173 in the text book.

16.11.1 Hazard Plotting

The hazard function is $F(t) = 1 - e^{-H(t)}$. Plot $(t, \widehat{H}(t))$ on the graph paper.

Example: Consider the exponential distribution. $t = -\frac{1}{\lambda}\log(1-F(t)) = -\frac{1}{\lambda}\log\left(e^{-H(t)}\right) = \frac{H(t)}{\lambda}$. Since $H(t) = \lambda t$ then regular graph paper can be used. $\widehat{H}(t)$ is well defined for censored data as well.

Example: The trial times are $t_1, t_2, t_3^+, t_4, t_5^+, ..., t_n$ and they have been ordered. $\widehat{h}(t) = \frac{1}{n}\frac{1}{n-1}\cdots-\frac{1}{n-3}\cdots-1$. $\widehat{H}(t) = \frac{1}{n}, \frac{1}{n}+\frac{1}{n-1}, \frac{1}{n}+\frac{1}{n-1}, \frac{1}{n}+\frac{1}{n-1}+\frac{1}{n-3}, \cdots$ Now, the theoretical $H(t|\theta)$ can be found for any distribution. We plot the points $[\widehat{H}(t|\widehat{\theta}), \widehat{H}_n(t)]$ for a linear relationship.

Example: Consider the example on page 176 of the text book. Remission time of 21 lukemia patients. Plotting $(t, \widehat{H}(t))$ is linear also. $H(t) = (\delta t)^\delta$, $\delta t = H(t)^{\frac{1}{\delta}}$, $t = \frac{1}{\lambda}H(t)^{\frac{1}{\delta}} = g(t)$.

16.12 Homework and Answers

Due October 18.

1. Do Exercise 5.1 on page 128 in the text book. Also, use the Cox-Mantel version of the test given in the class notes and check that the two expressions give the same result. Solution: For Gehan's test, the combined ordered set is

t_i	u_i
$\underline{3.9}$	-29
$\underline{5.4}$	-27
6.9	-25
7.7	-23
7.8^+	4
$\underline{7.9}$	-20
8.0	-18
8.2^+	6
8.2^+	6
8.3	-14
$\underline{10.5}$	-12
10.8^+	8
11.0^+	8
12.2^+	8
12.5^+	8
14.8^+	8
16.0^+	8
$\underline{16.6}^+$	8
$\underline{16.9}^+$	8
$\underline{17.1}^+$	8
18.1^+	8
$\underline{19.5}$	0
21.4^+	9
23.0^+	9
$\underline{23.8}^+$	9
24.4	5
24.8^+	10
26.9^+	10
$\underline{33.7}^+$	10
$\underline{33.7}^+$	10

$W = -29 - 27 - 20 - 12 + 8 + 8 + 8 + 0 + 9 + 10 + 10 = -35$. $n_1 = 11$, $n_2 = 19$.

$$\widehat{\sigma}_W^2 = \frac{n_1 n_2 \sum_{i=1}^{n_1+n_2} w_i^2}{(n_1+n_2)(n_1+n_2-1)} = \frac{11(19)}{30(29)}[(-29)^2 + (-27)^2 + \cdots + (10)^2] = 621.47$$

$z = \frac{W}{\hat{\sigma}_W} = \frac{-35}{\sqrt{621.47}} = -1.404$. $H_0 : s_1 = s_2$ versus $H_1 s_1 < s_2$. $-z_{0.05} = -1.64$. Therefore accept H_0. The table for the Cox-Mantel test is as follow. $r_1 = 5$ and $r_2 = 5$.

Distinct Failure Time	m_i	n_{1t}	n_{2t}	$r_{(i)}$	$A_{(i)}$
3.9	1	11	19	30	0.633
5.4	1	10	19	29	0.655
6.9	1	9	19	28	0.679
7.7	1	9	18	27	0.667
7.9	1	9	16	25	0.640
8.0	1	8	16	24	0.667
8.3	1	8	13	21	0.619
10.5	1	8	12	20	0.600
19.5	1	4	5	9	0.556
24.4	1	2	3	5	0.600

$U = r_2 - \sum_{i=1}^{k} m_{(i)} A_{(i)} = 5 - 6.316 = -1.316$.

$$I = \sum_{i=1}^{k} \frac{m_{(i)}(r_{(i)} - m_{(i)})}{r_{(i)} - 1} A_i(1 - A_{(i)}) = \left[\frac{1(30-1)}{29} 0.633(0.367) + \cdots\right] = 2.31357$$

$z = \frac{-1.316}{\sqrt{2.31357}} = -0.865$. $H_0 : s_1 = s_2$ versus $H_1 : s_1 < s_2$. $-z_{0.05} = -1.64$. Accept H_0. The following SAS code gives the results for the log rank test.

```
data melanoma;
input treatment survival censored;
cards;
1 33.7 0
1 3.9 1
1 10.5 1
1 5.4 1
1 19.5 1
1 23.8 0
1 7.9 1
1 16.9 0
1 16.6 0
1 33.7 0
1 17.1 0
2 8.0 1
2 26.9 0
2 21.4 0
2 18.1 0
2 16.0 0
2 6.9 1
2 11.0 0
2 24.8 0
2 23.0 0
2 8.3 1
2 10.8 0
2 12.2 0
2 12.5 0
2 24.4 1
2 7.7 1
```

```
2 14.8 0
2 8.2 0
2 8.2 0
2 7.8 0
;
run;

proc lifetest data=melanoma;
time survival*censored(0);
strata treatment;
run;
```

```
                          The SAS System                   14:16 Wednesday, December 31, 2008   1

                      The LIFETEST Procedure

                    Stratum 1: treatment = 1

                 Product-Limit Survival Estimates

                                                 Survival
                                                 Standard     Number      Number
      survival     Survival    Failure      Error      Failed        Left

        0.0000       1.0000          0           0         0          11
        3.9000       0.9091     0.0909      0.0867         1          10
        5.4000       0.8182     0.1818      0.1163         2           9
        7.9000       0.7273     0.2727      0.1343         3           8
       10.5000       0.6364     0.3636      0.1450         4           7
       16.6000*           .          .           .         4           6
       16.9000*           .          .           .         4           5
       17.1000*           .          .           .         4           4
       19.5000       0.4773     0.5227      0.1755         5           3
       23.8000*           .          .           .         5           2
       33.7000*           .          .           .         5           1
       33.7000*           .          .           .         5           0

         NOTE: The marked survival times are censored observations.


               Summary Statistics for Time Variable survival

                         Quartile Estimates

                           Point     95% Confidence Interval
               Percent    Estimate      [Lower      Upper)

                    75          .        19.5000          .
                    50     19.5000        7.9000          .
                    25      7.9000        3.9000          .

                      The LIFETEST Procedure

                         Mean    Standard Error

                      14.9273           2.1020

NOTE: The mean survival time and its standard error were underestimated because the largest observation was censored and the
                                  estimation was restricted to the largest event time.

                          The SAS System                   14:16 Wednesday, December 31, 2008   3

                      The LIFETEST Procedure

                    Stratum 2: treatment = 2

                 Product-Limit Survival Estimates

                                                 Survival
                                                 Standard     Number      Number
      survival     Survival    Failure      Error      Failed        Left

        0.0000       1.0000          0           0         0          19
        6.9000       0.9474     0.0526      0.0512         1          18
        7.7000       0.8947     0.1053      0.0704         2          17
        7.8000*           .          .           .         2          16
        8.0000       0.8388     0.1612      0.0854         3          15
        8.2000*           .          .           .         3          14
        8.2000*           .          .           .         3          13
        8.3000       0.7743     0.2257      0.1003         4          12
       10.8000*           .          .           .         4          11
       11.0000*           .          .           .         4          10
       12.2000*           .          .           .         4           9
       12.5000*           .          .           .         4           8
       14.8000*           .          .           .         4           7
       16.0000*           .          .           .         4           6
       18.1000*           .          .           .         4           5
       21.4000*           .          .           .         4           4
       23.0000*           .          .           .         4           3
       24.4000       0.5162     0.4838      0.2211         5           2
       24.8000*           .          .           .         5           1
       26.9000*           .          .           .         5           0

         NOTE: The marked survival times are censored observations.
```

```
                         The LIFETEST Procedure

               Summary Statistics for Time Variable survival

                           Quartile Estimates

                           Point     95% Confidence Interval
                Percent    Estimate      [Lower      Upper)

                     75       .          24.4000       .
                     50       .          24.4000       .
                     25     24.4000       8.0000       .


                           Mean    Standard Error

                        20.6441           1.8620

NOTE: The mean survival time and its standard error were underestimated because the largest observation was censored and the
                   estimation was restricted to the largest event time.

              Summary of the Number of Censored and Uncensored Values

                                                                       Percent
        Stratum       treatment       Total  Failed    Censored    Censored

              1               1          11       5           6       54.55
              2               2          19       5          14       73.68
        -------------------------------------------------------------------
          Total                          30      10          20       66.67

          Testing Homogeneity of Survival Curves for survival over Strata


                             Rank Statistics

                    treatment    Log-Rank    Wilcoxon

                    1              1.3150      35.000
                    2             -1.3150     -35.000


               Covariance Matrix for the Log-Rank Statistics

                  treatment             1             2

                  1               2.31384      -2.31384
                  2              -2.31384       2.31384


               Covariance Matrix for the Wilcoxon Statistics

                  treatment             1             2

                  1               1230.00      -1230.00
                  2              -1230.00       1230.00


                        Test of Equality over Strata

                                                  Pr >
                Test      Chi-Square      DF    Chi-Square

                Log-Rank      0.7474       1      0.3873
                Wilcoxon      0.9959       1      0.3183
                -2Log(LR)     0.3229       1      0.5699
```

$H_0 : \widehat{s}_1(t) = \widehat{s}_2(t)$ versus $H_1 : \widehat{s}_1(t) < \widehat{s}_2(t)$. Accept H_0 because the p value is 0.3873 which is insignificant.

2. Do Exercise 5.3 on page 128 in the text book. Carryout all of the tests including the test based on the PH model considered in class. The SAS code and output is as follow.

```
data tumor_free;
input diet $ survival censored;
cards;
lowfat 140 1
lowfat 177 1
lowfat 50 1
lowfat 65 1
lowfat 86 1
lowfat 153 1
lowfat 181 1
lowfat 191 1
lowfat 77 1
lowfat 84 1
```

```
lowfat 87 1
lowfat 56 1
lowfat 66 1
lowfat 73 1
lowfat 119 1
lowfat 140 0
lowfat 200 0
lowfat 200 0
lowfat 200 0
lowfat 200 0
lowfat 200 0
lowfat 200 0
lowfat 200 0
lowfat 200 0
lowfat 200 0
lowfat 200 0
lowfat 200 0
lowfat 200 0
lowfat 200 0
lowfat 200 0
saturatued 124 1
saturatued 58 1
saturatued 56 1
saturatued 68 1
saturatued 79 1
saturatued 89 1
saturatued 107 1
saturatued 86 1
saturatued 142 1
saturatued 110 1
saturatued 96 1
saturatued 142 1
saturatued 86 1
saturatued 75 1
saturatued 117 1
saturatued 98 1
saturatued 105 1
saturatued 126 1
saturatued 43 1
saturatued 46 1
saturatued 81 1
saturatued 133 1
saturatued 165 1
saturatued 170 0
saturatued 200 0
saturatued 200 0
saturatued 200 0
saturatued 200 0
saturatued 200 0
saturatued 200 0
unsaturated 112 1
unsaturated 68 1
unsaturated 84 1
unsaturated 109 1
```

```
unsaturated 153 1
unsaturated 143 1
unsaturated 60 1
unsaturated 70 1
unsaturated 98 1
unsaturated 164 1
unsaturated 63 1
unsaturated 63 1
unsaturated 77 1
unsaturated 91 1
unsaturated 91 1
unsaturated 66 1
unsaturated 70 1
unsaturated 77 1
unsaturated 63 1
unsaturated 66 1
unsaturated 66 1
unsaturated 94 1
unsaturated 101 1
unsaturated 105 1
unsaturated 108 1
unsaturated 112 1
unsaturated 115 1
unsaturated 126 1
unsaturated 161 1
unsaturated 178 1
;
run;


proc lifetest data=tumor_free;
time survival*censored(0);
strata diet;
run;
```

```
                         The SAS System                    13:18 Thursday, January 1, 2009  25

                       The LIFETEST Procedure

                     Stratum 1: diet = lowfat

                  Product-Limit Survival Estimates

                                          Survival
                                          Standard     Number      Number
    survival     Survival    Failure       Error       Failed       Left

       0.000       1.0000          0           0          0          30
      50.000       0.9667     0.0333      0.0328          1          29
      56.000       0.9333     0.0667      0.0455          2          28
      65.000       0.9000     0.1000      0.0548          3          27
      66.000       0.8667     0.1333      0.0621          4          26
      73.000       0.8333     0.1667      0.0680          5          25
      77.000       0.8000     0.2000      0.0730          6          24
      84.000       0.7667     0.2333      0.0772          7          23
      86.000       0.7333     0.2667      0.0807          8          22
      87.000       0.7000     0.3000      0.0837          9          21
     119.000       0.6667     0.3333      0.0861         10          20
     140.000       0.6333     0.3667      0.0880         11          19
     140.000*           .          .           .         11          18
     153.000       0.5981     0.4019      0.0899         12          17
     177.000       0.5630     0.4370      0.0912         13          16
     181.000       0.5278     0.4722      0.0920         14          15
     191.000       0.4926     0.5074      0.0924         15          14
     200.000*           .          .           .         15          13
     200.000*           .          .           .         15          12
     200.000*           .          .           .         15          11
     200.000*           .          .           .         15          10
     200.000*           .          .           .         15           9
     200.000*           .          .           .         15           8
     200.000*           .          .           .         15           7
     200.000*           .          .           .         15           6
     200.000*           .          .           .         15           5
```

```
200.000*          .          .          .        15          4
200.000*          .          .          .        15          3
200.000*          .          .          .        15          2
200.000*          .          .          .        15          1
200.000*          .          .          .        15          0

                    The SAS System                      13:18 Thursday, January 1, 2009  26

                 The LIFETEST Procedure

       NOTE: The marked survival times are censored observations.


            Summary Statistics for Time Variable survival

                         Quartile Estimates

                          Point     95% Confidence Interval
             Percent    Estimate      [Lower      Upper)

                  75        .           .            .
                  50     191.000     119.000         .
                  25      86.000      66.000     177.000


                         Mean    Standard Error

                      148.885           10.137

NOTE: The mean survival time and its standard error were underestimated because the largest observation was censored and the
                                     estimation was restricted to the largest event time.

                    The SAS System                      13:18 Thursday, January 1, 2009  27

                 The LIFETEST Procedure

                    Stratum 2: diet = saturatu

                  Product-Limit Survival Estimates

                                          Survival
                                          Standard     Number      Number
 survival     Survival    Failure          Error       Failed       Left

   0.000       1.0000          0              0          0           30
  43.000       0.9667     0.0333         0.0328          1           29
  46.000       0.9333     0.0667         0.0455          2           28
  56.000       0.9000     0.1000         0.0548          3           27
  58.000       0.8667     0.1333         0.0621          4           26
  68.000       0.8333     0.1667         0.0680          5           25
  75.000       0.8000     0.2000         0.0730          6           24
  79.000       0.7667     0.2333         0.0772          7           23
  81.000       0.7333     0.2667         0.0807          8           22
  86.000          .          .              .            9           21
  86.000       0.6667     0.3333         0.0861         10           20
  89.000       0.6333     0.3667         0.0880         11           19
  96.000       0.6000     0.4000         0.0894         12           18
  98.000       0.5667     0.4333         0.0905         13           17
 105.000       0.5333     0.4667         0.0911         14           16
 107.000       0.5000     0.5000         0.0913         15           15
 110.000       0.4667     0.5333         0.0911         16           14
 117.000       0.4333     0.5667         0.0905         17           13
 124.000       0.4000     0.6000         0.0894         18           12
 126.000       0.3667     0.6333         0.0880         19           11
 133.000       0.3333     0.6667         0.0861         20           10
 142.000          .          .              .           21            9
 142.000       0.2667     0.7333         0.0807         22            8
 165.000       0.2333     0.7667         0.0772         23            7
 170.000*         .          .              .           23            6
 200.000*         .          .              .           23            5
 200.000*         .          .              .           23            4
 200.000*         .          .              .           23            3
 200.000*         .          .              .           23            2
 200.000*         .          .              .           23            1
 200.000*         .          .              .           23            0

                    The SAS System                      13:18 Thursday, January 1, 2009  28

                 The LIFETEST Procedure

       NOTE: The marked survival times are censored observations.


            Summary Statistics for Time Variable survival

                         Quartile Estimates

                          Point     95% Confidence Interval
             Percent    Estimate      [Lower      Upper)

                  75     165.000     124.000         .
                  50     108.500      86.000     142.000
                  25      81.000      58.000      98.000


                         Mean    Standard Error

                      112.900            7.466

NOTE: The mean survival time and its standard error were underestimated because the largest observation was censored and the
                                     estimation was restricted to the largest event time.

                    The SAS System                      13:18 Thursday, January 1, 2009  29

                 The LIFETEST Procedure

                    Stratum 3: diet = unsatura
```

```
                   Product-Limit Survival Estimates

                                          Survival
                                          Standard     Number      Number
survival     Survival    Failure      Error       Failed       Left

   0.000       1.0000          0           0          0          30
  60.000       0.9667     0.0333      0.0328          1          29
  63.000            .          .           .          2          28
  63.000            .          .           .          3          27
  63.000       0.8667     0.1333      0.0621          4          26
  66.000            .          .           .          5          25
  66.000            .          .           .          6          24
  66.000       0.7667     0.2333      0.0772          7          23
  68.000       0.7333     0.2667      0.0807          8          22
  70.000            .          .           .          9          21
  70.000       0.6667     0.3333      0.0861         10          20
  77.000            .          .           .         11          19
  77.000       0.6000     0.4000      0.0894         12          18
  84.000       0.5667     0.4333      0.0905         13          17
  91.000            .          .           .         14          16
  91.000       0.5000     0.5000      0.0913         15          15
  94.000       0.4667     0.5333      0.0911         16          14
  98.000       0.4333     0.5667      0.0905         17          13
 101.000       0.4000     0.6000      0.0894         18          12
 105.000       0.3667     0.6333      0.0880         19          11
 108.000       0.3333     0.6667      0.0861         20          10
 109.000       0.3000     0.7000      0.0837         21           9
 112.000            .          .           .         22           8
 112.000       0.2333     0.7667      0.0772         23           7
 115.000       0.2000     0.8000      0.0730         24           6
 126.000       0.1667     0.8333      0.0680         25           5
 143.000       0.1333     0.8667      0.0621         26           4
 153.000       0.1000     0.9000      0.0548         27           3
 161.000       0.0667     0.9333      0.0455         28           2
 164.000       0.0333     0.9667      0.0328         29           1
 178.000            0     1.0000           0         30           0

                            The SAS System                      13:18 Thursday, January 1, 2009  30

                        The LIFETEST Procedure

            Summary Statistics for Time Variable survival

                          Quartile Estimates

                          Point     95% Confidence Interval
            Percent    Estimate      [Lower      Upper)

                 75     112.000     101.000     153.000
                 50      92.500      70.000     109.000
                 25      68.000      63.000      84.000


                          Mean    Standard Error

                        98.467             6.193


       Summary of the Number of Censored and Uncensored Values

                                                             Percent
   Stratum    diet          Total  Failed    Censored    Censored

         1    lowfat           30      15          15       50.00
         2    saturatu         30      23           7       23.33
         3    unsatura         30      30           0        0.00
   ---------------------------------------------------------------
     Total                     90      68          22       24.44

                            The SAS System                      13:18 Thursday, January 1, 2009  31

                        The LIFETEST Procedure

   Testing Homogeneity of Survival Curves for survival over Strata


                           Rank Statistics

                  diet        Log-Rank    Wilcoxon

                  lowfat       -14.768     -714.00
                  saturatu       0.969       37.00
                  unsatura      13.799      677.00


            Covariance Matrix for the Log-Rank Statistics

         diet           lowfat      saturatu      unsatura

         lowfat        15.6801       -9.3772       -6.3029
         saturatu      -9.3772       14.6563       -5.2791
         unsatura      -6.3029       -5.2791       11.5821


            Covariance Matrix for the Wilcoxon Statistics

         diet           lowfat      saturatu      unsatura

         lowfat        55839.7      -30196.9      -25642.8
         saturatu     -30196.9       53607.4      -23410.5
         unsatura     -25642.8      -23410.5       49053.3


                    Test of Equality over Strata
```

Test	Chi-Square	DF	Pr > Chi-Square
Log-Rank	20.7404	2	<.0001
Wilcoxon	12.3992	2	0.0020
-2Log(LR)	13.6909	2	0.0011

$H_0 : \widehat{s}_1(t) = \widehat{s}_2(t) = \widehat{s}_3(t)$ versus H_1 : one is not equal. Based on the test of equality over strata, we reject H_0. The next partial SAS output determines which diet is best out of the three. We are comparing the low fat diet versus the saturated diet.

Test of Equality over Strata

Test	Chi-Square	DF	Pr > Chi-Square
Log-Rank	4.7638	1	0.0291
Wilcoxon	3.7151	1	0.0539
-2Log(LR)	4.0697	1	0.0437

$H_0 : s_1 = s_3$ versus $s_1 > s_3$. Since the p-value is 0.0291, reject H_0. The low fat diet is better. Next, the saturated diet and the unsaturated diet will be compared.

Test of Equality over Strata

Test	Chi-Square	DF	Pr > Chi-Square
Log-Rank	5.3631	1	0.0206
Wilcoxon	2.5484	1	0.1104
-2Log(LR)	2.8359	1	0.0922

$H_0 : s_2 = s_3$ versus $s_2 > s_3$. Since the p-value is 0.0206, reject H_0. The saturated fat diet is better than the unsaturated fat diet. The low fat and the unsaturated fat diets are compared next.

Test of Equality over Strata

Test	Chi-Square	DF	Pr > Chi-Square
Log-Rank	21.7489	1	<.0001
Wilcoxon	12.4944	1	0.0004
-2Log(LR)	13.6326	1	0.0002

$H_0 : s_1 = s_3$ versus $H_1 : s_1 > s_3$. Since the p-value is 0.0001, we reject H_0. The low fat diet is better than the unsaturated fat diet. All-in-all, the low fat diet should be used when treating the re-ocurrance of the tumor. To obtain the PH model, the following SAS code must be added. Then, the corresponding output follows.

```
data tumor_free;
set tumor_free;
diet1 = 0;
diet2 = 0;
diet3 = 0;
if diet eq "lowfat" then diet1 = 1;
if diet eq "saturatu" then diet2 = 1;
if diet eq "unsatura" then diet3 = 1;
run;


proc phreg data = tumor_free;
model survival*censored(0) = diet1 diet2 diet3;
run;
```

```
                         The SAS System                    14:37 Thursday, January 1, 2009  12

                       The PHREG Procedure

                        Model Information

            Data Set                WORK.TUMOR_FREE
            Dependent Variable      survival
```

```
Censoring Variable       censored
Censoring Value(s)       0
Ties Handling            BRESLOW


Number of Observations Read         90
Number of Observations Used         90


Summary of the Number of Event and Censored Values

                                     Percent
    Total       Event    Censored   Censored

       90          68          22      24.44


             Convergence Status

 Convergence criterion (GCONV=1E-8) satisfied.


             Model Fit Statistics

                     Without           With
    Criterion     Covariates     Covariates

    -2 LOG L         539.009        519.099
    AIC              539.009        523.099
    SBC              539.009        527.538


                 The SAS System                      14:37 Thursday, January 1, 2009  13

               The PHREG Procedure

         Testing Global Null Hypothesis: BETA=0

 Test                 Chi-Square       DF     Pr > ChiSq

 Likelihood Ratio        19.9098        2         <.0001
 Score                   20.4568        2         <.0001
 Wald                    18.5110        2         <.0001


         Analysis of Maximum Likelihood Estimates

                    Parameter     Standard                                     Hazard
Variable    DF       Estimate        Error    Chi-Square    Pr > ChiSq          Ratio

diet1        1       -1.41646      0.33171       18.2348        <.0001          0.243
diet2        1       -0.63351      0.28250        5.0289        0.0249          0.531
diet3        0              0            .             .             .              .
```

The parameter estimates are

$$\underline{\widehat{\beta}} = \begin{pmatrix} -1.416466 \\ -0.633527 \\ 0 \end{pmatrix}$$

3. Do Exercise 5.7 in the text book. The sum of the ranks for treatment 1 are $\sum U_i = -273$. The sum of the ranks for treatment 2 are $\sum U_i = 170$ and the sum of the ranks for treatment 3 are $\sum U_i = 103$.

4. Do Exercise 5.8 in the text book. The sums for treatment 1 are $\sum = 10.65183$. The sums for treatment 2 are $\sum 19.34807$. $r_1 = 5, r_2 = 5$. $n_1 = 11, n_2 = 19$. $p = r_1 + r_2 = 10$. $\bar{t}'_1 = \frac{6.244201}{5} = 1.249$. $\bar{t}'_2 = \frac{5.88905}{5} = 1.17781$. $t_{(p+1)n} = 0.30483$.

$$\bar{t}_1 = \frac{5(1.249) + (11-5)(0.30483)}{5} = 1.6148$$

$$\bar{t}_2 = \frac{5(1.17781) + (19-5)(0.30483)}{5} = 2.0313$$

$F = \frac{\bar{t}_1}{\bar{t}_2} = \frac{1.6148}{2.0313} = 0.795$. $F_{0.975}(10,10) = 3.717$. $F_{0.025}(10,10) = 0.269$. H_0 : age means for each population are the same versus they are not (two sided test). Since $0.269 < 0.795 < 3.717$, we accept H_0.

5. Do Exercise 5.11 in the text book.

6. Let $x_{(r)}$ be the r^{th} order statistic in a sample of size n from an $\exp(\theta)$ distribution. Derive $E(x_{(r)})$.

7. Let $T_1, T_2, ..., T_n$ be the order statistics in a sample of size n from the Weibull distribution. Show that the $T_i's$ can be generated sequentially from

$$T_i = \frac{1}{\lambda}\left(\sum_{j=1}^{i} \frac{W_j}{(n-j+1)}\right)^{1/\delta}$$

where the $W_j's$ are independent and have standard exponential distributions.

8. Suppose two Weibull distributions have the same shape parameter but possibly different scale parameters. Show that the survivor functions are related by $s_1(t) = [s_2(t)]^{\delta}$. Give the explicit expression for δ. This serves as an example of the assumed survivor functions for the two groups in the PH model.

9. Consider the lung cancer data (standard, small). Using the PH model of Cox, carryout the test if $H_0 : \beta_j = 0$ is rejected or not for $j = 1, 2, 3, 4$. Now use only the covariates for which H_0 is rejected and give all parameter estimates, their standard error and $\widehat{s}(t)$. Also, compute $\widehat{s}(t|\underline{x})$ for three of the $\underline{x}$ values in the table and plot these three for different t.

16.13 Goodness-of-Fit Tests

For the mid-term exam, you may bring one 3" $\times$ 5" note card with one side of notes only. You must answer 5 out of 6 questions. The mid-term will be from 9:30 to 11:30 am.

This section will cover tests about the assumed distribution for the survival function. The null hypothesis is $H_0 : F(t) = F_0(t)$. For uncensored case: the test for the exponential distribution is as follow. Let the random variable T be the survival time. We wish to test $H_0 : T \sim \exp(\theta)$ where θ is unknown. Let $t_1, t_2, ..., t_n$ be a random sample. $WE_1 = \frac{\sum_{i=1}^{n}(t_i-\bar{t})^2}{\left(\sum_{i=1}^{n} t_i\right)^2}$. It is used because $E(T) = \theta$ and $Var(T) = \theta^2$. Then, $WE_1 = \frac{S^2}{\bar{t}^2}\frac{1}{n}$, $S^2 = \frac{1}{n}\sum_{i=1}^{n}(t_i - \bar{t})^2$. The distribution of WE_1 does not depend on θ if H_0 is true. Proof: Take $t_i^* = \frac{t_i}{\theta}$, $T_i^* \sim \exp(1)$. But, $WE_1 = \frac{\sum_{i=1}^{n}(t_i-\bar{t})^2}{\left(\sum_{i=1}^{n} t_i\right)^2} = \frac{\sum_{i=1}^{n}(t_i^*-\bar{t}^*)^2}{\left(\sum_{i=1}^{n} t_i^*\right)^2} \Rightarrow$ the distribution WE_1 does not depend on θ under H_0. Critical points are given in Table C8 in the text book. For the exponential distribution, $Var(T) = [E(T)]^2$. But for other distributions, $Var(T) \leq [E(T)]^2$. Therefore, reject H_0 if WE_1 if it is too large or too small.

Example: Consider the example on page 183 of the text book. $WE_1 = 0.025$, $n = 21$. The 95% confidence interval is $(0.02, 0.085)$. Therefore, accept H_0.

The test for the two parameter exponential distribution is $H_0 : F(T) = \frac{1}{\theta}e^{-\frac{(T-G)}{\theta}}$, $T > G$. If $t_1 < t_2 < \cdots < t_n$ is the ordered sample, then $E(T) = \theta + G$ and $\widehat{G} = t_1$ and $\widehat{\theta} = \bar{t} - t_1$. The variance is still θ^2. $s^2 = \sum_{i=1}^{n}\frac{(t_i-\bar{t})^2}{n}$. $WE_2 = \frac{(\bar{t}-t_1)^2}{\sum_{i=1}^{n}(t_i-\bar{t})^2} = \frac{1}{n}\frac{(\bar{t}-t_1)^2}{s^2}$. $\widehat{\theta}$ is the mle of $\theta \Rightarrow \widehat{\theta}^2$ is the mle for θ^2. Table C9 in the text book gives the confidence intervals.

The test for the normal (and the log-normal) distribution will be given next. Suppose that the random variable T equals to the survival time. If T is log-normal then $X = \log T \sim N(\mu, \sigma^2)$. Let $t_1 < t_2 < \cdots < t_n$ be an ordered sample. $x_1, x_2, ..., x_{n-1}, x_n$ is an order sample from a normal distribution. For the normal distributions, $\widehat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$ is the mle.

$$K = \begin{cases} \frac{n}{2}, & \text{if } n \text{ is even.} \\ \frac{n-1}{2}, & \text{if } n \text{ is odd.} \end{cases}$$

$b = \sum_{i=1}^{K} a_{n-i+1}(x_{n-i+1} - x_i)$ is an estimator of σ. Table C10 in the text book gives the $a_i's$. Then b^2 is an estimator of σ^2. $W = \frac{b^2}{\sum_{i=1}^{n}(x_i-\bar{x})^2} = \frac{1}{n}\frac{\tilde{\sigma}^2}{\hat{\sigma}^2}$. Table C11 in the text book gives the cut-off points. We reject for small values of W because the range (at the tails) is larger than that of other distributions. For large n, $Z = \delta + \eta\frac{\log(w-\epsilon)}{1-w)} \to N(0,1)$ where δ, η, ϵ are fixed constants for a given n. See Table C12 in the text book.

16.13.1 Pearson Chi-Square Goodness-of-Fit

We wish to test the hypothesis $H_0 : x \sim f(x|\theta)$ where θ is a parameter vector. A random sample is $x_1, x_2, ..., x_n$. The Pearson test is a test for the multinomial distribution. $p_i(\theta) = P(c_{i-1} < x < c_i) = \int_{c_{i-1}}^{c_i} f(x|\theta)\,dx$. Then, classify $(x_1, x_2, ..., x_n)$ to $(n_1, n_2, ..., n_k)$ where n_i equals to the number of $(x_1, x_2, ..., x_n)$ lying in the interval (c_{i-1}, c_i). Then, $n_1, n_2, ..., n_k \sim multinomial(n, p_1, p_2, ..., p_k)$. $X^2 = \frac{\sum_{i=1}^{k}(n_i - np_i(\theta))^2}{np_i(\theta)} = \frac{(O_i-E_i)^2}{E_i}$, where $E(n_i) = np_i(\theta)$ and $O_i = n_i$. If H_0 is such that $\theta = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_r \end{pmatrix}$ is known, then $X^2 \to \chi^2(k-1)$ as $n \to \infty$. Reject H_0 if $X^2 > \chi^2_\alpha(k-1)$. In practical terms, we know θ. If θ is unknown, let $\widehat{\theta}$ be the mle based on the multinomial distribution or minimum chi-square estimator which minimizes X^2. Then, $\widehat{X}^2 = \sum_{i=1}^{k} \frac{(n_i - np_i(\widehat{\theta}))^2}{np_i(\widehat{\theta})} \to \chi^2(k-r-1)$ as $n \to \infty$. The wrong estimator comes from $L = \prod_{i=1}^{n} f(x_i|\theta)$. You should use the likelihood function

$$L = \frac{n!}{\prod_{i=1}^{n} n_i!}\prod_{i=1}^{n} p_i(\theta)^{n_i}$$

which is the multinomial likelihood function. It is less efficient. Let $\tilde{\theta}$ be the mle based on $x_1, x_2, ..., x_n$. $\tilde{X} = \frac{\sum(n_i - np_i(\tilde{\theta}))^2}{np_i(\tilde{\theta})}$. So, if you do not reject $\tilde{X}^2$, then you will not reject H_0 based on $\widehat{X}^2$. But, if $\tilde{X}^2$ is in the rejection region, then $\widehat{X}^2$ has to be computed. If $\tilde{X}^2$ is used instead of $\widehat{X}^2$, then the real α, say α^* is higher than α. Page 190 in the text book uses the wrong estimator. k is arbitrary. The text book author suggests using $k = 4\left[\frac{2(n-1)^2}{z_\alpha^2}\right]^{\frac{1}{5}}$ given in Equation 7.29 is too large.

16.13.2 Goodness-of-Fit for Censored Data

Let a sample be $t_1 < t_2 < \cdots < t_n$. The hypothesis being tested is $H_0 : s(t) = s_0(t)$ is a specified function. Hollander and Proschan use

$$\widehat{s}(t) = \prod_{\text{all } it_i \le t} \frac{n-i}{n-i+1}$$

where t_i are uncensored.

$$\widehat{f}(t_i) = \widehat{s}(t_{i-1}) - \widehat{s}(t_i) = \frac{1}{n}\prod_{j=1}^{i-1}\left(\frac{n-j+1}{n-j}\right)^{1-\delta_j}$$

where

$$\delta_i = \begin{cases} 1, & \text{if uncensored.} \\ 0, & \text{otherwise.} \end{cases}$$

The test statistic is given by $c = \sum_{i=1}^{n} s_0(t_i)\widehat{f}(t_i)$, $c^* = \frac{\sqrt{n}(c-\frac{1}{2})}{\widehat{\sigma}} \to N(0,1)$. $\widehat{\sigma}^2 = \frac{1}{16}\sum_{i=1}^{n}\frac{n}{n-i+1}\left(s_0^4(t_{i-1}) - s_0^4(t_i)\right)$. On page 193, Table 7.6 for example, reject H_0 if $|c^*| > z_{\frac{\alpha}{2}}$.

Exponential Distribution without Censoring

Consider the exponential distribution. If $X \sim \exp(\lambda)$, then $2\lambda X \sim \chi^2(2)$. $f(x) = \lambda e^{-\lambda x}$, $x > 0$. $\mu = E(x) = \frac{1}{\lambda}$. For $f(x) = \frac{1}{\theta} e^{-\frac{x}{\theta}}$, $\mu = \theta$. The mle is $\widehat{\lambda} = \frac{1}{\bar{t}}$ in the first pdf. The mle is $\widehat{\mu} = \bar{t}$ in the second pdf. Also, $2\lambda \sum_{i=1}^n t_i \sim \chi^2(2n) = \frac{2\sum_{i=1}^n t_i}{\mu}$. Also, $\frac{2n\bar{t}}{\mu} = \frac{2n\widehat{\mu}}{\mu} \sim \chi^2(2n)$.

$$1-\alpha = P\left(\chi^2(2n, 1-\alpha/2) < \frac{2n\widehat{\mu}}{\mu} < \chi^2(2n, \alpha/2)\right) \Rightarrow \left(\frac{2n\widehat{\mu}}{\chi^2(2n, \alpha/2)}, \frac{2n\widehat{\mu}}{\chi^2(2n, 1-\alpha/2)}\right)$$

is a $(1-\alpha)100\%$ confidence interval.

Exponential Distribution with Censoring

Under the sampling plan with censoring, we stop at the r^{th} observation. The likelihood function is

$$L = \frac{n!}{(n-r)!} \left(\prod_{i=1}^r \lambda e^{-\lambda t_i}\right) e^{-(n-r)\lambda t_r}$$

The mle of λ is

$$\widehat{\lambda} = \frac{r}{\sum_{i=1}^r t_i + (n-r)t_r}.$$

Helprin (1952) shows for large n, r that $\frac{2r\widehat{\mu}}{\mu}$ is approximately $\chi^2(2r)$. In the censored sampling design, we can also stop at a fixed time T. In this case, the likelihood function becomes

$$L = \frac{n!}{(n-r)!} \left(\prod_{i=1}^r \lambda e^{-\lambda T_i}\right) e^{-\lambda(n-r)T}$$

$$\widehat{\lambda} = \frac{r}{\sum_{i=1}^r t_i + (n-r)T},$$

$$\widehat{\mu} = \frac{\sum_{i=1}^r t_i + (n-r)T}{r}.$$

Exponential Distribution with Progressive Censoring

Let T_i equal to the time that the i^{th} observation is on trial. For the censored observation, $T_i = t_i^+$. Let the data be $t_1 < t_2 < \cdots < t_r$ and $t_1^+, t_2^+, ..., t_{n-r}^+$. The likelihood function

$$L = c\left(\prod_{i=1}^r \lambda e^{-\lambda t_i}\right) \prod_{i=1}^{n-r} e^{-\lambda t_i^+}.$$

The mle of λ is

$$\widehat{\lambda} = \frac{r}{\sum_{i=1}^r t_i + \sum_{i=1}^{n-r} t_i^+}.$$

Also, $\sqrt{n}(\widehat{\lambda} - \lambda) \to N(0, \sigma_\lambda^2)$ where

$$\sigma_\lambda^2 = \frac{n\lambda^2}{\sum_{i=1}^n (1 - e^{-\lambda T_i})}.$$

$$Var(\widehat{\lambda}) = \frac{\lambda^2}{\sum_{i=1}^n (1 - e^{-\lambda T_i})}$$

$$\widehat{\mu} = \frac{1}{\widehat{\lambda}},\ \ Var(\widehat{\mu}) = \frac{\mu^2}{\sum_{i=1}^{n}(1-e^{-\lambda T_i})} \Rightarrow \frac{\frac{(\widehat{\mu}-\mu)}{\mu}}{\sqrt{\sum_{i=1}^{n}(1-e^{-\lambda T_i})}} \to N(0,1) =$$

$$\left(\frac{\widehat{\mu}}{\mu}-1\right)\left(\sum_{i=1}^{n}(1-e^{-\lambda t_I})\right)^{-\frac{1}{2}} \to N(0,1).$$

The latter expression is used to find the confidence interval of μ.

Exponential Distribution (Two Parameter Family)

In addition to the scale parameter, the two parameter exponential family distribution has a location parameter G. The pdf is $f(x) = \lambda e^{-\lambda(x-G)}$, $x > G$, $\lambda > 0$. Suppose the data is $t_1, t_2, ..., t_n$ is the ordered sample. The likelihood function is

$$L = n!\lambda^n e^{-\lambda\sum_{i=1}^{n}(t_i-G)} = n!\lambda^n e^{-\lambda\sum_{i=1}^{n}t_i+n\lambda G}$$

is true for $G < t_1 < t_2 < \cdots < t_n < \infty$. We need to estimate λ and G. Note that $L \uparrow$ of G. The mle of G is $\widehat{G} = t_1$. $\frac{d\log L}{d\lambda} = 0 \Rightarrow \lambda = \frac{n}{\sum_{i=1}^{n}(t_i-G)} \Rightarrow \widehat{\lambda} = \frac{n}{\sum_{i=1}^{n}(t_i-t_1)}$. $X - G \sim \exp(\lambda)$. $Y = X - G \sim (\lambda) \Rightarrow E(X) = E(Y) + G = \frac{1}{\lambda} + G$. $\mu = E(X) = \frac{1}{\lambda} + G$. $\widehat{\mu} = \frac{1}{\widehat{\lambda}} + \widehat{G} = \frac{\sum_{i=1}^{n}(t_i-t_1)}{n} + t_1 = \sum_{i=1}^{n}\frac{t_i-nt_1+nt_1}{n} = \bar{t}$. The formulas on page 208 of the text book are wrong because $2\lambda T_i$ is not $\chi^2(2)$ but $2\lambda(T_i - G) \sim \chi^2(2)$.

For the censoring case where we stop at the r^{th} observation, the likelihood function is

$$L = \frac{n!}{(n-r)!}\left(\prod_{i=1}^{r}\lambda e^{-\lambda(T_i-G)}\right)e^{-(n-r)(t_r-G)\lambda},\ t_1 < t_2 < \cdots < t_r.$$

$\widehat{G} = t_1$ and $\widehat{\lambda} = \frac{r}{\sum_{i=1}^{r}(t_i-t_1)+(n-r)(t_r-t_1)}$. Note that $\sum_{i=1}^{r}(t_i-t_1)+(n-r)(t_r-t_1) = \sum_{i=1}^{r}t_i-nt_1+(n-r)t_r = \sum_{i=2}^{r}(n-i+1)(t_i-t_{i-1})$ which is the total survival time observed between the first and the r^{th} observations. $\mu = \frac{1}{\lambda} + G$ and $\theta = \frac{1}{\lambda}$. $\widehat{\theta} = \frac{1}{\widehat{\lambda}} = \sum_{i=2}^{r}\frac{(n-i+1)(t_i-t_{i-1})}{r} = \sum_{i=2}^{r}\frac{Y_i}{r}$ where $Y_i = (n-i+1)(t_i-t_{i-1})$. $y_2, y_3, ..., y_r$ are iid $\exp(\lambda)$. Prove that G is not involved. It cancels out. $E(\widehat{\theta}) = \frac{(r-1)E(Y_i)}{r} = \frac{(r-1)\theta}{r}$. $\tilde{\theta} = \sum_{i=2}^{r}\frac{(n-i+1)(t_i-t_{i-1})}{r-1}$ is unbiased. Now $E(\tilde{\theta}) = \theta$. Find the estimator of $\widehat{G}$. $\widehat{G} = t_1$, $(t_1 - G)\sum\exp(n\lambda)$. t_1 has a delayed exponential distribution with parameters G and $n\lambda$. $E(t_1) = \frac{1}{n\lambda} + G \Rightarrow \widehat{G} = t_1$ is biased for G. $E(t_1) = \frac{\theta}{n} + G$. $\tilde{\theta}$ is unbiased for θ. $\tilde{G} = t_1 - \frac{\tilde{\theta}}{n}$. $E(\tilde{G}) = E(t_1) - E\left(\frac{\tilde{\theta}}{n}\right) = \frac{\theta}{n} + G - \frac{\theta}{n} = G \Rightarrow \tilde{G}$ is unbiased for G. $\mu = \frac{1}{\lambda} + G$. $\mu = \theta + G$. An unbiased estimator for μ is $\tilde{\mu} = \tilde{\theta} + \tilde{G} = \tilde{\theta} + t_1 - \frac{\tilde{\theta}}{n} = \frac{(n-1)}{n}\tilde{\theta} + t_1 = \tilde{\mu}$. Note that $T^* = \sum_{i=2}^{r}Y_i$ is such that $2\lambda T^* \sim \chi^2[2(r-1)]$ and can be used for the confidence interval of $\theta = \frac{1}{\lambda}$. For $G = 0$, we have $\theta = \mu$.

Confidence Interval of G

We know that $\widehat{G} = t_1$. $(t_1 - G) \sim \exp(n\lambda)$ and it is independent of T^*. $2n\lambda(t_1 - G) \sim \chi^2(2)$. $2\lambda T^* \sim \chi^2[2(r-1)]$. If $X \sim \chi^2(r_1)$ and $Y \sim \chi^2(r_2)$ and X, Y are independent then $\frac{X/r_1}{Y/r_2} \sim F(r_1, r_2)$. So,

$$\frac{2n\lambda(t_1-G)/2}{2\lambda T^*/[2(r-1)]} \sim F[2, 2(r-1)].$$

A $(1-\alpha)100\%$ confidence interval of G is $t_1 - \frac{\tilde{\theta}}{n}F_\alpha[2, 2(r-1)] < G < t_1$.

Delayed Exponential Distribution

We know that for estimation purposes $\tilde{G} = t_1 - \frac{\tilde{\theta}}{n}$ where $\tilde{\theta} = \frac{T^*}{r-1}$ and $\tilde{\lambda} = \frac{1}{\tilde{\theta}}$. $T^* = \sum_{i=2}^{r}(n-i+1)(t_i - t_{i-1}) = \sum_{i=2}^{r} x_i$, where the $x_i's$ are iid $x_i \sim \exp(\lambda)$. $Var(\tilde{\theta}) = Var\left(\frac{T^*}{r-1}\right) = \frac{1}{(r-1)^2}(r-1)\theta^2 = \frac{\theta^2}{r-1}$. x_i are independent of t_1. T^* is independent of T_1. $Var(\tilde{G}) = Var(T_1) + \frac{1}{n^2}Var(\tilde{\theta}) = \frac{\theta^2}{n^2} + \frac{\theta^2}{n^2(r-1)} = \frac{\theta^2}{n}\frac{r}{r-1}$ because $T_1 \sim \exp(\lambda n)$ and $\theta = \frac{1}{\lambda}$.

Weibull Estimation

$t_1, t_2, ..., t_n$ is the random sample. The likelihood function is

$$L = \delta^n \lambda^{n^\delta} \left(\prod_{i=1}^{n} t_i\right)^{\delta-1} \exp\left\{-\lambda^\delta \sum_{i=1}^{n} t_i^\delta\right\}$$

$(t_1, t_2, ..., t_n)$ is the minimum set of sufficient statistics. The mle is $\log L = n\log\delta + n\delta\log\lambda + \sum_{i=1}^{n}(\delta - 1)\log t_i - \lambda^\delta \sum_{i=1}^{n} t_i^\delta$. Taking the usual derivatives with respect to the parameters, $\frac{d\,\log L}{d\,\delta}$, $\frac{d\,\log L}{d\,\lambda} = 0 \Rightarrow n - \lambda^\delta \sum t_i^\delta = 0$, and $\Rightarrow \frac{n}{\delta} + n\log\lambda + \sum \log t_i - \lambda^\delta \sum t_i^\delta(\log\lambda + \log t_i) = 0$. Solving the first equation for λ yields $\lambda = \left(\frac{n}{\sum t_i^\delta}\right)^{\frac{1}{\delta}}$. δ must be solved numerically using all three expressions derived so far.

For the case of singularly censored data, stop at the r^{th} failure. $t_1 < t_2 < \cdots < t_r < t_{r+1}^+, t_{r+2}^+, ..., t_n^+ = t_r$. The likelihood function is

$$L = c\delta^r \lambda^{\delta r} \left(\prod_{i=1}^{r} t_i\right)^{\delta-1} \exp\left\{-\lambda^\delta \sum_{i=1}^{r} t_i^\delta\right\} \exp\left\{-(n-r)\lambda^r t_r^\delta\right\}.$$

The mle equations are

$$r + \lambda^\delta \left(\sum_{i=1}^{r} t_i^\delta + (n-r)t_r^\delta\right) = 0,$$

$$\frac{r}{\delta} + r\log\lambda + \sum_{i=1}^{r}\log t_i - \lambda^\delta \left[\sum_{i=1}^{r} t_i^\delta(\log\lambda + \log t_i) + (n-r)t_r^\delta(\log\lambda + \log t_r)\right] = 0$$

Solve the first equality for λ.

For the progressively censored case, the same is $t_1, t_2, ..., t_r, t_{r+1}^+, ..., t_n^+$. In the above mle, replace $(n-r)t_r^\delta$ by $\sum_{i=r+1}^{n} t_i^\delta$ in the first equality. In the second equality with zero, replace $(n-r)t_r^\delta(\log\lambda + \log t_r)$ by $\sum_{i=r+1}^{n} t_i^\delta(\log\lambda + \log t_i)$.

Log-Normal Distribution Estimation

For the random variable T to be log-normal means $\log T \sim N(\mu, \sigma^2)$. Let $t_1, t_2, ..., t_n$ be a random sample from a log normal distribution.

$$f(t) = \frac{1}{\sqrt{2\pi}\sigma t} e^{-\frac{(\log t - \mu)^2}{2\sigma^2}},\ t > 0.$$

$$\mu_T = \exp\{\mu + \frac{1}{2}\sigma^2\},\ \ \sigma_T^2 = (e^{\sigma^2} - 1)\exp\{2\mu + \sigma^2\}.$$

Proof: Let $x_i = \log t_i$. Then, $x_1, x_2, ..., x_n$ is a normal random sample. Maximum likelihood gives $\widehat{\mu} = \bar{x}$, and $\widehat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2 = s_x^2$. The mle of μ_T is $\widehat{\mu}_T = \exp\{\bar{x} + \frac{1}{2}s_x^2\}$, and the mle of σ_T is $\widehat{\sigma}_T =$

$(e^{s_x^2}-1)\exp\{2\bar{x}+s_x^2\}$. To find the bias, we need $E(\widehat{\mu}_T)$ and $E(\widehat{\sigma}_T^2)$. That is left for a homework problem.

In the censored case where we stop at the r^{th} success, the pdf is

$$F(x)=\frac{1}{\sqrt{2\pi}\sigma}\int e^{-\frac{(u-\mu)^2}{2\sigma^2}},du.$$

The likelihood function is

$$L=c\prod_{i=1}^{r}f(x_i)\prod_{i=r+1}^{n}[1-F(x_i^+)].$$

For the case where we stop at the r^{th} observation (see Sarhan and Greenberg), the best linear estimators for $t_1,t_2,...,t_r$; $(t_{r+1}^+=\cdots=t_n^+=t_r)$ are $\tilde{\mu}=\sum_{i=1}^r a_i\log t_i$ and $\tilde{\sigma}=\sum_{i=1}^r b_i\log t_i$ where a_i and b_i are constants given in Table C-14 of the text book. a_i and b_i increase as i increases. t_r gets the largest weight. An approximate mle by Cohen (1961) for μ and σ^2 are $\widehat{\mu}=\bar{x}-\widehat{\lambda}(\bar{x}-\log t_r)$ and $\widehat{\sigma}^2=s_x^2+\widehat{\lambda}(\bar{x}-\log t_r)^2$ where $\bar{x}=\frac{1}{r}\sum_{i=1}^r x_i$ and $s_x^2=\frac{1}{r}\sum_{i=1}^r(x_i-\bar{x})^2$. $\widehat{\lambda}$ is tabulated.

Gamma Distribution Estimation

The pdf of the gamma distribution is

$$f(t)=\frac{\lambda^\delta}{\Gamma(\delta)}e^{-\lambda t}t^{\delta-1}.$$

The likelihood function is

$$L=\frac{\lambda^{n\delta}e^{-\lambda\sum_{i=1}^n t_i}\left(\prod_{i=1}^n t_i\right)^{\delta-1}}{(\Gamma(\delta))^n}.$$

$m_1=\sum_{i=1}^n t_i$ and $m_2=\prod_{i=1}^n t_i$ are the sufficient statistics for (λ,δ). $\log L=n\delta\log\lambda-\lambda m_1+(\delta-1)\log m_2-n\log\Gamma(\delta)$. The mle equations are $\frac{d\,\log L}{d\,\lambda}=0\Rightarrow\lambda=\frac{n\delta}{m_1}$. Using this in $\frac{d\,\log L}{d\,\delta}=0\Rightarrow\frac{\Gamma(\delta)'}{\Gamma(\delta)}-\log\delta-\log m_2^{\frac{1}{n}}+\log\frac{m_1}{n}=0$ where $\Gamma(\delta)'=\frac{d\,\Gamma(\delta)}{d\,\delta}$. Tables exist for this solution for a given $R=\frac{nm_2^{\frac{n}{n}}}{n_1}$ because $g(\delta)=\log R$.

The moment estimators are $E(T)=\frac{\delta}{\lambda}$ and $Var(T)=\frac{\delta}{\lambda^2}$. $\bar{t}=\frac{\delta}{\lambda}$ and $s^2=\frac{\delta}{\lambda^2}\Rightarrow\tilde{\delta}=\frac{\bar{t}^2}{s_t^2}$ and $\tilde{\lambda}=\frac{\bar{t}}{s_t^2}$.

The bias correcting estimators are as follow. Let $\widehat{\theta}$ be biased for θ. $E(\widehat{\theta})=\theta+b_n(\theta)$. If $\widehat{b}_n$ is unbiased for $b_n(\theta)$, then $\tilde{\theta}=\widehat{\theta}-\widehat{b}_n$ is unbiased for θ. If $b_n(\widehat{\theta})$ is not unbiased for $b_n(\theta)$, then $\tilde{\theta}=\widehat{\theta}-b_n(\widehat{\theta})$ is a *biased reducing estimator.* Let $E(\widehat{\theta})=\theta+\frac{1}{n}b(\theta)+\Theta\left(\frac{1}{n^2}\right)$. Now, the bias reducing estimator is $\tilde{\theta}=\widehat{\theta}-\frac{1}{n}b(\widehat{\theta})$. For the gamma distribution, there are some bias correcting mle. Let $\widehat{\delta}$ be the mle of δ.

$$\widehat{\delta}_c=\frac{\widehat{\delta}}{1+\frac{\zeta}{n}},\quad\widehat{\lambda}=\frac{\widehat{\delta}_c}{\bar{t}}\left(1-\frac{1}{n\widehat{\delta}_c}\right)$$

are bias reducing estimators. $E(\widehat{\delta})\simeq\delta\left(1+\frac{\zeta}{n}\right)+\Theta\left(\frac{1}{n^2}\right)\Rightarrow\widehat{\delta}_c=\frac{\delta}{\left(1+\frac{\zeta}{n}\right)}$.

Next, consider the gamma distribution under the censored sampling design. Let $t_1<t_2<\cdots<t_r<t_{r+1}^+=\cdots=t_n^+=t_r$ be a random sample. Let $\eta=\lambda t_r$.

$$m=\frac{\left(\prod_{i=1}^r t_i\right)^{\frac{1}{\delta}}}{t_r}\text{ and }s=\sum_{i=1}^r\frac{t_i}{rt_r}.$$

The mle equations are $\log m=\frac{n}{r}\frac{\Gamma(\delta)'}{\Gamma(\delta)}-\frac{n}{r}\log\eta-\left(\frac{n}{r}-1\right)\frac{J'}{J}$. $s=\frac{\delta}{\eta}-\frac{1}{\eta}\left(\frac{n}{r}-1\right)\frac{e^{-\eta}}{J}$ where $J=\int_1^\infty t^{\delta-1}e^{-\eta t}\,dt$. $J'=\frac{d\,J}{d\,\delta}=\int_1^\infty t^{\delta-1}\log te^{-\eta t}\,dt$.

16.14 Homework 3 Goes Here

Do problems 6.7, 7.6, 8.6, 9.1, 9.2, 10.5, 11.4. Find the bias of the mle of the log normal mean and variance. Find $E(X)$ and $Var(X)$.

16.15 Regression Methods for Distribution Fitting

The mle for censored data are involved. To estimate the hazard function, equate the non-parametric estimator function of $h(t)$ with the assumed parametric function. $\widehat{h}(t_i)$ is the non-parametric estimator of $h(t)$.

1. Exponential distribution — $h(t) = \lambda$, $\lambda > 0$, $t > 0$.
2. Weibull distribution — $h(t) = \lambda'\delta t^{\delta-1}$, $\lambda', \delta > 0$, $\lambda' = \lambda^\delta$.
3. Gompers distribution — $h(t) = \exp\{\lambda + \delta t\}$, $-\infty < \lambda < \infty$, $\delta > 0$.
4. Linear exponential distribution — $h(t) = \lambda + \delta t$, $\lambda > 0$, $\delta \exists h(t) > 0$.

When $\delta = 0$ in (2)-(4), it implies an exponential model in (1). Suppose we have the regression model $y_i = a + bx_i + e$ where $y_i = f(\widehat{h}(t_i))$.

Model	y_i	a	b	x
(1)	$\widehat{h}(t_i)$	λ	0	$---$
(2)	$\log \widehat{h}(t_i)$	$\log(\lambda'\delta)$	$\delta - 1$	$\log t_i$
(3)	$\log \widehat{h}(t_i)$	λ	δ	t_i
(4)	$\log \widehat{h}(t_i)$	λ	δ	t_i

For the exponential distribution, $\widehat{h}(t_i) = \lambda + e_i$.

Example: Consider the model in (2). $y_i = a + bx_i + e_i \equiv \log h(t) = a + bx$, $\log \widehat{h}(t) = a + bx + e$. Minimize $\sum_{i=1}^{s}(y_i - a - bx_i)^2$ for the estimated parameters a and b. Here $t_1, t_2, ..., t_s$ are uncensored observations. Finally, we solve for $\widehat{\lambda}$ and $\widehat{\delta}$.

16.15.1 Weighted Least Squares Estimator

We wish to minimize $\sum w_i(y_i - a - bx_i)^2$ where the weights w_i are as follow.

	w_i
(1)	1
(2)	$\frac{1}{V_i}$
(3)	$n_i b_i$

n_i equals to the number at risk in the i^{th} interval for classified data. b_i equals to the width of the interval. $\widehat{V_i} = Var[\widehat{h}(t_i)]$. How do we choose the weights? One way is to look at $\widehat{L}(\widehat{\lambda}, \widehat{\delta})$ for which one gives the maximum. Another way is to look at the residuals of $\sum_{i=1}^{s} w_i(y_i - \widehat{a} - \widehat{b}x_i)^2$. Here $\widehat{a} = \bar{y}' - \widehat{b}\bar{x}'$.

$$\widehat{b} = \frac{\sum_{i=1}^{s} w_i(y_i - \bar{y}')(x_i - \bar{x}')}{\sum_{i=1}^{s} w_i(x_i - \bar{x}')^2}$$

where

$$\bar{x}' = \frac{\sum_{i=1}^{s} w_i x_i}{\sum_{i=1}^{s} w_i}, \quad \bar{y}' = \frac{\sum_{i=1}^{s} w_i y_i}{\sum_{i=1}^{s} w_i}.$$

For classified data, find an estimator of the likelihood function

$$L = c\prod_{i=1}^{s-1}\left[1-\frac{\widehat{s}(t_{i+1})}{\widehat{s}(t_i))}\right]^{d_i}\left[\frac{\widehat{s}(t_{i+1})}{\widehat{s}(t_i)}\right]^{n_i'-d_i}$$

where $n_i' = n_i$ minus the number lost during the i^{th} interval where n_i equals the number at risk at the i^{th} interval and d_i equals to the number of deaths in the i^{th} interval.

Model	
(1)	$\widehat{s}(t) = e^{-\widehat{\lambda}t}$
(2)	$\widehat{s}(t) = e^{-(\widehat{\lambda}t)^{\widehat{\delta}}}$
(3)	$\exp\{-\frac{\exp((\widehat{\lambda})}{\widehat{\delta}}(\exp(\widehat{\delta}t)-1)\}$
(4)	$\widehat{s}(t) = \exp\{-\widehat{\lambda}t + \frac{1}{2}\widehat{\delta}t^2\}$

Let's compare the exponential fit with the other three models. $H_0 : T \sim \exp(\lambda) \Rightarrow H_0 : \delta = 0$. $H_1 : T \sim model(j)$, $j = 2,3,4 \Rightarrow \delta \neq 0$. Use the likelihood ratio test to test the hypotheses. $\widehat{L}(j)$ equals the maximum of $L(j)$ for model j. Because of the number of parameters, $\widehat{L}(1) \leq \widehat{L}(j)$, $j = 2,3,4$. The test is based on

$$2\log\left(\frac{\widehat{L}(j)}{\widehat{L}(1)}\right) = -2\log\left(\frac{\widehat{L}(1)}{\widehat{L}(j)}\right) \sim \chi^2(1).$$

If this is not significant, then do not reject H_0. The exponential distribution is a good fit.

16.15.2 Chi-Square Test for the Fit of a Given Model

Let the empirical likelihood function $\widehat{L}(j)$ be the maximum of $L(j)$ for model j. Let $\widehat{L}$ be the non-parametric Kaplan-Meir estimator of L. Let there be s intervals.

$$-2(\log\widehat{L}(j) - \log\widehat{L}) = -2\log\left(\frac{\widehat{L}(j)}{\widehat{L}}\right) \to \chi^2(s-1-k)$$

where k equals to the number of parameters in the j^{th} model. $H_0 : T \sim distribution(j)$ versus $H_1 : \widehat{L} > \widehat{L}(t)$ because $\widehat{L}$ has s parameters and $\widehat{L}(t)$ only has 2 parameters.

$$-2\log\left(\frac{\widehat{L}(j)}{\widehat{L}}\right) = 2\log\left(\frac{\widehat{L}}{\widehat{L}(j)}\right).$$

Reject H_0 if

$$2\log\left(\frac{\widehat{L}}{\widehat{L}(j)}\right) \geq \chi^2_\alpha(s-1-k).$$

Suppose $s(t) = e^{-(\lambda t)^\delta}$. See Figure ??. The benefits are

1. $s(t)$ can be estimated at any point.
2. We are estimating a less number of parameters.

Example: Consider example 8.12 on page 229 of the text book. This is the survival data for plasma cell myeloma. Under the model

$$2\log\left(\frac{\widehat{L}(j)}{\widehat{L}(1)}\right),\ \ j=2,3,4$$

all are significant. Therefore, the exponential model is not a good fit. $\widehat{h}(t)$ for the Weibull distribution increases to 0.0317 at 2.75 months. Medical knowledge says it should not increase that fast. Therefore, select Gompers with the weight $w_i=\frac{1}{\widehat{V}_i}$. The selection for $\widehat{L}$ for the weights $w_i=\frac{1}{\widehat{V}_i}$ are as follow.

		Model Preference
Weibull	-226.52	(1)
Gompers	-226.90	(3)
Log-Linear	-226.77	(2)

16.16 Comparing Two Survival Distributions

The likelihood ratio test tests $X\sim f(x|\theta)$, $\theta\in\Omega$, $\theta'=(\theta_1,\theta_2,...,\theta_k)$, where $\Omega: k$ dimensional parameter space. The null hypothesis is $H_0:\theta\in\Omega_0\subset\Omega$, $\Omega_0: r$ dimensional parameter space $r<k$, $k-r$ equals to the number of parameters specified by H_0. $x_1,x_2,...,x_n$ is a random sample. The likelihood function is $L(\theta|\underline{x})=\prod_{i=1}^n f(x_i|\theta)$. Let $\widehat{\theta}$ be the mle of θ. Also, let $\widehat{\theta}_0$ be the mle of θ under the null hypothesis H_0.

$$0\le\lambda=\frac{L(\widehat{\theta}_0|\underline{x})}{L(\widehat{\theta}|\underline{x})}\le 1$$

We reject H_0 for small values of λ. Sometimes $\lambda\le c\Rightarrow T\in A$. If the distribution of T is known, then we can carry out the test based on T. For large n, $-2\log\lambda\to\chi^2(k-r)$. We reject H_0 if $-2\log\lambda\ge\chi^2_\alpha(k-r)$. Suppose that $X\sim\exp(\lambda_1)$ and $Y\sim\exp(\lambda_2)$. We test the null hypothesis $H_0:\lambda_1=\lambda_2=\lambda$. This also says that $s_1(t)=s_2(t)$. We are not testing whether or not the distributions are exponential or not exponential. Assuming censoring, a sample is $x_1,x_2,...,x_{r_1},x^+_{r+1},...,x^+_{n_1}$ and $y_1,y_2,...,y^+_{r_2},...,y^+_{n_2}$. The likelihood function is

$$L(\lambda_1,\lambda_2|\underline{xy})=\lambda_1^{r_1}e^{-\lambda_1\sum_{i=1}^{r_1}x_i}e^{-\lambda_1\sum_{i=r_1+1}^{n_1}x_i^+}\lambda_2^{r_2}e^{-\lambda_2\sum_{i=1}^{r_2}y_i}e^{-\lambda_2\sum_{i=r_2+1}^{n_2}y_i^+},$$

$$\frac{d\log L}{d\lambda_1}=0\Rightarrow\widehat{\lambda}_1=\frac{r_1}{\sum_{i=1}^{r_1}x_i+\sum_{i=r_1+1}^{n}x_i^+}\quad\frac{d\log L}{d\lambda_2}=0\Rightarrow\widehat{\lambda}_2=\frac{r_2}{\sum_{i=1}^{r_2}y_i+\sum_{i=r_2+1}^{n}y_i^+}.$$

Under the null hypothesis H_0, $\frac{d\log L(\lambda,\lambda|\underline{xy})}{d\lambda}=0\Rightarrow$

$$\widehat{\lambda}=\frac{r_1+r_2}{\sum_{i=1}^{r_1}x_i+\sum_{i=1}^{r_2}y_i+\sum_{i=r_1+1}^{n}x_i^++\sum_{i=r_2+1}^{n}y_i^+}$$

The ratio has a chi-square distribution.

$$\Lambda=\frac{L(\widehat{\lambda},\widehat{\lambda}|\underline{xy})}{L(\widehat{\lambda}_1,\widehat{\lambda}_2|\underline{xy})},\ \ -2\log\Lambda\to\chi^2(k-r)=\chi^2(1).$$

We reject H_0 if $-2\log\Lambda>\chi^2_\alpha(1)$.

Example: This is Example 5.1 from the text book. The treatment is CMF. The sample is $23, 16^+, 18^+, 20^+, 24^+$. The control is $15, 18, 19, 19, 20$. $n_1 = n_2 = 5$. $r_1 = 1$ and $r_2 = 5$. $-2\log\Lambda = 3.344$. $\chi^2_{0.05}(1) = 3.84$. Thus, we do not reject H_0.

Consider the model where $X \sim \exp(\lambda_1)$ and $Y \sim \exp(\lambda_2)$. Cox's F test for the exponential distribution for *uncensored* data $t_{11}, t_{12}, ..., t_{1n_1} \sim \exp(\lambda_1)$ and $t_{21}, t_{22}, ..., t_{2n_2} \sim \exp(\lambda_2)$. Then,

$$\frac{\lambda_1 \sum_{i=1}^{n_1} t_{1i}}{\lambda_2 \sum_{i=1}^{n_2} t_{2i}}$$

is the ratio of two gamma distributions and they are independent. $H_0 : \lambda_1 = \lambda_2$. The ratio becomes the test statistic. For censored data, $x_1, x_2, ..., x_{r_1}, x^+_{r_1+1}, ..., x^+_{n_1}$, and $y_1, y_2, ..., y_{r_2}, y^+_{r_2+1}, ..., y^+_{n_2}$.

$$\bar{t}_1 = \frac{\sum_{i=1}^{r_1} x_i + \sum_{i=r_1+1}^{n_1} x_i^+}{r_1} = \frac{1}{\widehat{\lambda}_1}, \quad \bar{t}_2 = \frac{1}{\widehat{\lambda}_2}.$$

Cox (1953) suggests the test $\frac{\bar{t}_1}{\bar{t}_2} = \frac{\widehat{\lambda}_2}{\widehat{\lambda}_1}$ is approximately $F(2r_1, 2r_2)$. Suppose $H_1 : \lambda_1 > \lambda_2$. We reject H_0 if $\frac{\bar{t}_1}{\bar{t}_2} < F_{1-\alpha}(2r_1, 2r_2)$. Suppose $H_1 : \lambda_1 < \lambda_2$. We reject H_0 if $\frac{\bar{t}_1}{\bar{t}_2} > F_\alpha(2r_1, 2r_2)$. The confidence interval of $\frac{\lambda_2}{\lambda_1}$ is derived as

$$\frac{\lambda_1 \bar{t}_1}{\lambda_1 \bar{t}_2} \sim F(2r_1, 2r_2) \Rightarrow 1 - \alpha = P\left(a < \frac{\lambda_1 \bar{t}_1}{\lambda_2 \bar{t}_2} < b\right),$$

$a = F_{1-\alpha/2}(2r_1, 2r_2)$ and $b = F_\alpha(2r_1, 2r_2)$.

$$P\left(a\frac{\bar{t}_2}{\bar{t}_1} < \frac{\lambda_1}{\lambda_2} < b\frac{\bar{t}_2}{\bar{t}_1}\right)$$

16.16.1 Testing About Two Weibull Distributions

The pdf for two Weibull distributions is $f_i(t) = \lambda_i \delta_i (\lambda_i t)^{\delta_i - 1} e^{-(\lambda_i t)^{\delta_i}}$, $i = 1, 2$. We wish to test $H_0 : \lambda_1 = \lambda_2$ and $\delta_1 = \delta_2 \Rightarrow s_1(t) = s_2(t)$.

$$\Lambda = \frac{L(\widehat{\lambda}, \widehat{\delta} | \underline{xy})}{L(\widehat{\lambda}_1 \widehat{\lambda}_2, \widehat{\delta}_1 \widehat{\delta}_2 | \underline{xy})}, \quad -2\log\Lambda \to \chi^2(k - r), \quad k - r = 2.$$

Testing for $\delta_1 = \delta_2$ assuming that $\lambda_1 = \lambda_2$ is known, the test statistic is $\frac{\widehat{\delta}_1}{\widehat{\delta}_2}$. Thomas and Baine (1969) simulated the distribution of $\frac{\widehat{\delta}_1}{\widehat{\delta}_2}$ under $H_0 : \delta_1 = \delta_2$. See Table C-18 in the text book. $H_1 : \delta_1 > \delta_2$. We reject H_0 if $\frac{\widehat{\delta}_1}{\widehat{\delta}_2} > \ell_\alpha$. If we do not reject H_0, then we can test $H_0 : \lambda_1 = \lambda_2$. The test statistic is $G = \frac{1}{2}\left(\widehat{\delta}_1 + \widehat{\delta}_2\right)(\log\widehat{\lambda}_2 - \log\widehat{\lambda}_1)$ assuming that $\delta_1 = \delta_2$. The distribution is given in Table C-19 of the text book.

Example: This is Example 9.3 in the text book. It simulates data from a $Weibull(\delta, \lambda)$ distribution. $\delta_1 = 2, \lambda_1 = 0.01$. $\delta_2 = 3, \lambda_2 = 0.01$. $n_1 = n_2 = 40$. We test $H_0 : \delta_1 = \delta_2$ versus $H_1 : \delta_2 > \delta_1$. Reject H_0 if $\frac{\widehat{\delta}_2}{\widehat{\delta}_1} > \ell_\alpha$. So, $\frac{\widehat{\delta}_2}{\widehat{\delta}_1} = 1.396$, $\ell_{0.05} = 1.342$. Therefore reject H_0.

16.16.2 Comparing Two Gamma Distributions

Suppose that $X \sim Gamma(\lambda_1, \delta_1)$ and $Y \sim Gamma(\lambda_2, \delta_2)$. For uncensored samples, $H_0 : \lambda_1 = \lambda_2$ assuming δ_1 and δ_2 are known. If $n_1 = n_2$, then the Rao (1952) test is $\frac{\bar{x}}{\bar{y}} \sim F(2n\delta_1, 2n\delta_2)$ under H_0. If $H_1 : \lambda_1 > \lambda_2$, then reject H_0. $\frac{\bar{x}}{\bar{y}} \sim \frac{\lambda_2}{\lambda_1} F(2n\delta_1, 2n\delta_2)$. If $H_1 : \lambda_2 > \lambda_1$, then reject H_0 if $\frac{\bar{x}}{\bar{y}} < F_{1-\alpha}(2n\delta_1, 2n\delta_2)$.

16.17 A Regression Problem

On Wednesday, December 3^{rd} there will be a guest speaker on the Cornfield paper. This will be a 40 minute talk.

Consider survival functions depending on other variables or hazard functions depending on other variables. We can look at graphs of the hazard function or the survival function for the single variable effect.

Example: Let T equal to the survival time for pediatric acute lukemia. Other variables include:

- Age at diagnosis.
- Histologic type (structure of tissue) ALL, AUL, AML.
- Initial white blood count at diagnosis.

Cox's PH model for survival is $h(t|x) = h_0(t)\exp\{x\beta\}$. The likelihood function is

$$L(\beta|x) = \prod_{i=1}^{k} \frac{e^{x_{(i)}\beta}}{\sum_{\ell \in R_i} e^{x_{i(\ell)}\beta}}$$

Suppose there are two age groups. $H_0 : s_1(t) = s_2(t)$. Use the Cox model with

$$x_1 = \begin{cases} 0, & \text{if in group 1.} \\ 1, & \text{if in group 2.} \end{cases}$$

Then test $H_0 : \beta = 0$.

16.17.1 Two Sample Problem with Time Dependent Covariates

Before we had $h_1(t) = h_0(t)e^{x_1\beta_1}$, $x_1 = 0, 1$. Now, we have $h(t) = h_0(t)e^{(\beta_1+\beta_2 t)x_1}$. $h_1(t) = h_0(t)e^{(\beta_1+\beta_2 t)} = e^{\beta_1}h_0(t)e^{\beta_2 t}$. In $h_1(t)$, the effect is different at different times. $\frac{h_1(t)}{h_0(t)} = e^{\beta_1+\beta_2 t}$ is not a constant. This is also called the *relative risk.* Before, relative risk was a constant. $H_0 : \beta_2 = 0$ implies that relative risk is a constant. The regression problem is as follow. Let $\log\left(\frac{h_i(t)}{h_0(t)}\right) = y_i$ where $h_i(t) = h_0(t)e^{x_i\beta}$ which is the hazard function for the i^{th} individual. $y_i = \sum_{j=1}^{p} x_{ij}\beta_j$. Here, y_i is not observed directly or independently.

Example: Let

$$x_1 = \begin{cases} 1, & \text{if patient is hypertensive.} \\ 0, & \text{otherwise.} \end{cases}$$

$x_1 = 0$ provides the control group. $x_1 = 1$ is the treatment group. $h_1(t) = h_0(t)e^{\beta_1}$. $\frac{h_1(t)}{h_0(t)} = e^{\beta_1}$ equals to the relative risk. Let (β_{1L}, β_{2U}) be the confidence interval of β_1. Then, $(e^{\beta_1 L}, e^{\beta_2 U})$ is the confidence interval of e^{β_1}.

$$P\left(\beta_{1L} < \beta_1 < \beta_{2U}\right) = P\left(e^{\beta_1 L} < e^{\beta_1} < e^{\beta_2 U}\right) = 1 - \alpha.$$

It is similar to finding the shortest confidence interval of the log normal distribution. $(e^{\beta_1 L}, e^{\beta_2 U})$ is not the shortest interval even if $(\beta_1 L, \beta_2 U)$ is the shortest interval.

Suppose there are x variables. Then, we use *stepwise regression.* The procedure is as follow. Let there be p variables.

1. Select variable x_i if $L(\widehat{\beta}_i) \geq L(\widehat{\beta}_j)$, $j = 1, 2, ..., p$.

2. Select the j^{th} variable at the second stage if $L(\widehat{\beta}_i, \widehat{\beta}_j) \geq L(\widehat{\beta}_i, \widehat{\beta}_k)$, $k = 1, 2, ..., p$.

At each step, test if $H_0 : \beta_k = 0$. Then, $-2[\log L(\widehat{\beta}_1, ..., \widehat{\beta}_{k-1}) - \log L(\widehat{\beta}_1, ..., \widehat{\beta}_k)] \sim \chi^2(1)$.

Example: This example is on page 259 of the text book. As k increases, $L(\widehat{\beta}_1, ..., \widehat{\beta}_k)$ increases. Look at the likelihood ratio test to see if at each stage if L is increasing significantly. $H_0 : \beta_k = 0$.

Example: This is example 10.2 on page 257 of the text book. This is survival data for 30 patients with AML.

$$x_1 = \begin{cases} 1, & \text{if age} > 50. \\ 0, & \text{otherwise.} \end{cases}$$

$$x_2 = \begin{cases} 1, & \text{if C. of marrow clot is 100\%.} \\ 0, & \text{otherwise.} \end{cases}$$

$h(t) = h_0(t)e^{\beta_1 x_1 + \beta_2 x_2}$. We are testing $H_0 : \beta_1 = 0$ and $H_0 : \beta_2 = 0$. The relative risk of age equals

$$\frac{[h(t)]_{x_1=1, x_2=0}}{[h(t)]_{x_1=x_2=0}} = e^{\beta_1}.$$

The relative risk of both factors equals

$$\frac{[h(t)]_{x_1=x_2=1}}{h_0(t)} = e^{\beta_1+\beta_2}.$$

The regression table is

	$\widehat{\beta}_i$	Std Error	p-value	$e^{\widehat{\beta}_i}$
x_1	1.01	0.46	0.013	2.75
x_2	0.35	0.44	0.212	1.42

$H_0 : \beta_2 = 0$, $z = \frac{0.35}{0.44}$ implies do not reject H_0. The confidence interval for e^{β_1} is $1.12 < e^{\beta_1} < 6.75$.

Stratification

Now we will stratify with respect to a variable.

Stratum 1 Age ≥ 50.
Stratum 2 Age < 50.

$h_{0i}(t)$ are different for $i = 1, 2$. $h_i(t|x) = h_{0i}(t)\exp\{\sum \beta_j x_j\}$, $i = 1, 2$. Earlier when age was one of the x variables, we assume $\frac{h(t|x_1 \geq 50)}{h(t|x_1 < 50} = c$ is a constant. But now, that is not the case.

16.17.2 Parametric Regression Models

On November 13, 1997 Dr Peter D'Neal will give a lecture from 1:00 to 1:30 at BAL room 107. On Monday November 24, Dr Justine Shults will give a lecture during class time on Cox's PH model.

Consider a log linear exponential stratified population. We have k groups. n_i equals to the number of observations from the i^{th} group. $n = \sum n_i$. There are p covariates $x_{ij\ell_j}$, $i = 1, 2, ..., k$, $j = 1, 2, ...n_i$, $\ell = 1, 2, ..., p$. $s_{ij}(t) = e^{-\lambda_{ij} t}$, $i = 1, 2, ..., k$; $j = 1, 2, ..., n_i$. λ_{ij} is different for each person. The number of parameters equals to the number of observations. Therefore, we need to assume a model for λ_{ij}. Assume that $\lambda_{ij} = e^{a_i + \sum_{\ell=1}^{p} b_\ell x_{ij\ell}}$. Now, the number of parameters equals $k+p$. $x_{ij\ell}$ are transformed such that the smallest value for each i is zero. Then, e^{a_i} equals to the treatment effect. $e^{b_\ell x_{ij\ell}}$ equals to the effect of the ℓ^{th} covariate. b_ℓ determines the effect of the ℓ^{th} covariate. $b_\ell = 0 \Rightarrow \ell^{th}$ covariate is not significant. For censored data,

$$L = \prod_{i=1}^{k}\prod_{j=1}^{n_i} (\lambda_{ij})^{\delta_{ij}} e^{-\lambda_{ij} t_{ij}}$$

where λ_{ij} is given in the model above.

$$\log L(a,b) = \sum\sum[\delta_{ij}(a_i + \sum b_\ell x_{ij\ell}) - t_{ij}\exp\{a_i + \sum_\ell b_\ell x_{ij\ell}\}]$$

$\gamma_i = \sum_j \delta_{ij}$ where

$$\delta_{ij} = \begin{cases} 1, & \text{if not censored.} \\ 0, & \text{if censored.} \end{cases} \quad = \text{ number of uncensored observations from the } i^{th} \text{ group.}$$

$s_{ij} = \sum_j \delta_{ij} x_{ij\ell} =$ sum of the $x's$ from the i^{th} group for the uncensored observations. Then, $\frac{d \log L}{d\, a_i} = 0$ and $\frac{d \log L}{d\, b_\ell} = 0$ imply $\gamma_i - e^{a_i}\sum_j t_{ij}\exp\{\sum_\ell b_\ell x_{j\ell}\} = 0$, $i = 1,2,...,k$. $\sum_i [s_{i\ell} - e^{a_i}\sum_j t_{ij} x_{ij\ell}\exp\{\sum_\ell b_\ell x_{ij\ell}\}] = 0$, $\ell = 1,2,...,p$. Then, $L(\widehat{a},\widehat{b}) = \max_{a,b} L$. $H_0 : b_1 = b_2 = \cdots = b_p = 0$. We test H_0 based on the likelihood ratio test $-2[\log L(\widehat{a},0) - \log L(\widehat{a},\widehat{b})] \to \chi^2(p)$ if H_0 is true. This is equal to $-2\log\left(\frac{\widehat{L}_0}{\widehat{L}_1}\right) = 2\log\left(\frac{\widehat{L}_1}{\widehat{L}_0}\right)$. We reject for large values only. To test to see if the groups are different, $H_0 : a_1 = a_2 = \cdots = a_k = a$. $-2\log[L(\tilde{a},\tilde{b}) - L(\widehat{a},\widehat{b})] \to \chi^2(k-1)$. If H_0 about $\underline{b} = 0$ is rejected, the a stepwise selection gives $-2\log[L(\widehat{a},\widehat{b}_i) - \log(\widehat{a},0)]$, $i = 1,2,...,b$.

Example: This is example 10.5 on pages 266-68 of the text book using stepwise regression. $n = 268$ patients going through chemotherapy. There are 7 different treatments. Randomize the patients into 7 groups. The covariates are initial white blood cell count (WBC), and age at diagnosis. $x_1 = \log WBC$. $x_2 =$ age. $x_3 = (age)^2$. The table on page 268 of the text book gives the analysis. x_1 is the most significant. All the variables x_1, x_2, x_3 significantly affect the survival function. Taken x_2 and x_3 alone in the model, the coefficient of x_2 changes to a negative number. Consider the transformation $x_1 = \frac{(WBC^{\theta_1}}{\theta_1} \to \log(WBC)$ as $\theta_1 \to 0$. $x_3 = x_2^{\theta_2}$, $\theta_2 > 1$. θ_1 and θ_2 are to be estimated.

16.17.3 Linear Exponential Model of Feigl and Zelen

We have n patients (no groups) and p covariates. x_{ij}, $i = 1,...,n$. $j = 1,2,...,p$. $s_i(t) = e^{-\frac{t}{\lambda_i}}$, $i = 1,2,...,n$. $\mu_i = \frac{1}{\lambda_i} = b_0 + b_1 x_{i1} + \cdots + b_p x_{ip}$. Now the number of parameters equals to $p+1$. $\mu_i = \sum_{j=0}^{p} b_j x_{ij}$ and $x_{i0} = 1, \forall i$. If all $x_{ij} = 0$, $j = 1,2,...,p$, then $\mu_i = \frac{1}{\lambda_i} = b_0$. The base hazard function is $h_0(t) = \frac{1}{b_0}$. The likelihood function (uncensored) is

$$L(b) = \prod_{i=1}^{n}\lambda_i e^{-\lambda_i t_i} = \prod_{i=1}^{n}\left(\sum_{j=1}^{p} b_j x_{ij}\right)^{-1}\exp\left\{-\sum_i t_i\left(\sum_j b_j x_{ij}\right)^{-1}\right\}$$

because $\lambda_i = \left(\sum_j b_j x_{ij}\right)^{-1}$. The mle equations now are $\frac{d \log L}{d\, b_i} = 0$, $j = 0,1,...,p$.

$$-\sum_i x_{ij}\left(\sum_\ell b_\ell x_{i\ell}\right)^{-1} + \sum_i t_i x_{ij}\left(\sum_\ell b_\ell x_{i\ell}\right)^{-2} = 0, j = 0,1,...,p.$$

The survival function is $\widehat{s}_i(t) = e^{-\widehat{\lambda}_i t} = \exp\{-t\sum_{j=0}^{p}\widehat{b}_j x_{ij}\}$ is the estimate of the survival function for the i^{th} individual. We test the null hypothesis $H_0 : b_1 = b_2 = \cdots = b_p = 0$.

16.17.4 A Chi Square Test

Testing for the exponential model $\lambda_i = \left(\sum_j b_j x_{ij}\right)^{-1}$, we wish to estimate the $(100p)^{th}$ percentile $t_i(p)$ for the i^{th} person. $\widehat{s}(t_i(p)) = \exp[(-t_i(p))\left(\sum_j b_j x_{ij}\right)^{-1}] = 1 - p$. Do it for $p_1, p_2, ..., p_k$. $t_i(p_j)$, $i = 1, 2, ..., n$; $j = 1, 2, ..., k$.

Class	1	2	$\cdots$	k
Observations	n_1	n_2	$\cdots$	n_k
Expected	np_1	np_2	$\cdots$	np_k

$$\sum \frac{(n_i - np_i)^2}{np_i} \rightarrow \chi^2[k - (p+1)].$$

Example: This example is on page 271 of the text book. These are the patients with AML.

Quantiles1	2	3	4	
Observations5	4	3	5	
Expected	4.25	4.25	4.25	4.25

$X^2 = 0.317 \Rightarrow$ not significant $\Rightarrow$ the model fits. Use $\chi^2(4-2-1) = \chi^2(1)$.

16.17.5 Linear Exponential of Byer et al

$\lambda_i = \sum_j b_j x_{ij}$. We have censored data. There are r observations and $s = n - r$ censored observations. Then, the likelihood function is

$$L = \prod_{i=1}^{r} \lambda_i e^{-\lambda_i t_i} \prod_{i=1}^{s} e^{-\lambda_i t_i^+} = \prod \left(\sum b_j x_{ij}\right) e^{-\sum b_j x_{ij} t_i} \prod_{i=1}^{s} e^{-\sum b_j x_{ij} t_i^+}.$$

$$\frac{d \log L}{d\, b_\ell} = 0 \Rightarrow \sum \left[\frac{x_{i\ell}}{\sum_j b_j x_{ij}} - x_{i\ell} t_i\right] - \sum_{k=1}^{s} x_{k\ell} t_k^+ = 0, \ell = 1, 2, ..., p.$$

If x_{ij} are binary random variables (i.e. 0 or 1), then we are just summing th $b's$.

Example: This is example 10.7 on page 276 of the text book. The condition is prostate cancer. The sample size is $n = 1824$. x_{ij} are binary random variables. All variables except number 1 are significant. $\widehat{b}_j > 1.96$. There are 5 risk groups. $\widehat{s}(t_i) = e^{-\widehat{\lambda}_i t_i}$. Compare this with the observed $\widehat{s}(t)$ (i.e. the Kaplan-Mier estimator).

16.17.6 Identification of Risk Factors

Example: Is family history an important risk factor for breast cancer? Other factors include age, race, number of pregnancies, experience of breast feeding, use of contraceptives, etc. H_i : history level i, $i = 1, 2, ..., k$. In the ideal setting, P(cancer with $H_i|$ all other factors fixed). Consider the problem of comparing the risk variables of two groups. The univariate model uses the z test for binomials or the t test for continuous data. The example on page 283 of the text book shows a test for responders and non-responders.

Odds Ratio and the Chi Square Test

Consider the presence or absence of the risk factor as a ratio. E = present, $\bar{E}$ = absent. For a treatment, S = present, and $\bar{S}$ = absent.

	E	$\bar{E}$	Totals
S	a	b	R_1
$\bar{S}$	c	d	R_2
	c_1	c_2	N

$X^2 = \sum_{i=1}^{2}\sum_{j=1}^{2}\frac{(O_{ij}-E_{ij})^2}{E_{ij}}$ where $E_{ij} = \frac{R_i c_j}{N} = \frac{ad-bc}{R_1R_2c_1c_2}$. OR = odds ratio = the ratio of two odds.

$$OR = \frac{P(S|E)/P(\bar{S}|E)}{P(S|\bar{E})/P(\bar{S}|\bar{E})}, \quad \widehat{OR} = \frac{\frac{a}{c_1}/\frac{c}{c_1}}{\frac{b}{c_2}/\frac{d}{c_2}} = \frac{ad}{bc}.$$

The presence of risk factor E is beneficial if $\widehat{OR} > 1$. It is harmful if $\widehat{OR} < 1$.

Example: This is example 11.2 in the text book. E is age < 50.

	E	$\bar{E}$	
Response	27	10	
Non-Response	12	22	71

$\widehat{OR} = 4.95 \Rightarrow$ age is a significant risk factor.

Linear Discriminate Function

Suppose there are two groups denoted by 1 and 2 (success and failure). Let X be measurements of p risk variables on an individual. $y = \sum_{j=1}^{p} b_j x_j = b^T X$ is called the *linear discriminant function* if it can be used to classify the subject in one of the two groups.

Definition: Given two p-variate normal populations $N(\mu_1, \Sigma)$ and $N(\mu_2, \Sigma)$, the linear discriminant function (log of ratios of two densities, apart from a constant) is given by

$$c + y = \log\left[\frac{f(x|\mu_1\Sigma)}{f(x|\mu_2\Sigma)}\right]$$

Then, $y = (\mu_1 - \mu_2)^T\Sigma^{-1}X = b^T X$ where $b^T = (\mu_1-\mu_2)^T\Sigma^{-1}$. We need to estimate μ_1, μ_2, and Σ. x_{ijk}, $i = 1, 2$; $j = 1, 2, ..., n_i$; $k = 1, 2, ..., p$. $\bar{x}_{ik} = \sum_j \frac{x_{ijk}}{n_i}$. $a_{k\ell} = \frac{\sum\sum(x_{ijk}-\bar{x}_{ik})(x_{ij\ell}-\bar{x}_{i\ell})}{n_1+n_2-2}$. $s = \{a_{ij}\}_{p\times p}$. Let $s^{-1} = \{s_{ij}\} = B$. The mle of b is $\widehat{b}^T = (\bar{X}_1 - \bar{X}_2)^T B$. $\widehat{b}_j = \sum_k d_k s_{jk}$ where $d_k = \bar{X}_{1k} - \bar{X}_{2k}$. Then, $y = \widehat{b}^T X$, $y_i = \sum_k \widehat{b}_k \bar{X}_{ik}$, $i = 1, 2$. $\bar{y}_i$ equals to the estimated average value of the linear discriminant function for the i^{th} group. $y_0 = \frac{\bar{y}_1+\bar{y}_2}{2}$. Suppose we get a new patient. How do we assign X? $y = \widehat{b}^T X$. The new y is assigned to group 2.

Accuracy of the Discriminant Function

The assignment by the discriminant function is according to the following table.

	1	2	
1	n_{11}	n_{12}^*	n_1
2	n_{21}^*	n_{22}	n_2
			n

The values n_{12} and n_{21} are wrongly assigned. The error proportions are $\frac{n_{12}}{n_1}$ and $\frac{n_{21}}{n_2}$. Another criterion to check the accuracy using

$$d^2 = \frac{(\bar{y}_1 - \bar{y}_2)^2}{\text{pooled within group variance of } y} = \frac{\bar{y}_1 - \bar{y}_2)^2}{\sum_{i=1}^{2}\sum_{j=1}^{n_i}(y_{ij} - \bar{y}_i)^2/(n_1 + n_2 - 2)}.$$

Then, $\sqrt{d^2} = d$ is known as the *generalized distance* between two populations. We want large values for d to reject on $H_0 : E(\bar{y}_1) = E(\bar{y}_2)$.

Mahalanobis Distance

The Mahalanobis distance function is another measure of accuracy. $H_0 : \mu_1 = \mu_2$ for $\underline{x}$. $D^2 = (\bar{x}_1 - \bar{x}_2)^T S^{-1}(\bar{x}_1 - \bar{x}_2)$. If H_0 is true, then

$$\frac{n_1 n_2(n_1 + n_2 - p - 1)D^2}{p(n_1 + n_2)(n_1 + n_2 - 2)} \sim F(p, r)$$

where $r = n_1 + n_2 - p - 1$. If H_0 is accepted, we cannot use the discriminant function.

16.17.7 Logistic Regression Method

The data comes in the success or failure of a treatment.

$$y_i = \begin{cases} 1, & \text{if } i^{th} \text{ is success.} \\ 0, & \text{otherwise.} \end{cases}$$

Also, we have p covariates which may affect the chance of success. $P_i = P(y_i = 1|x_{i1}, x_{i2}, ..., x_{ip})$. If we assume that $P_i = \sum_{j=1}^{p} b_j x_{ij}$, $0 < p_i < 1$ is hard to control. Therefore, this will not work. Using logistic regression,

$$P_i = \frac{\exp\{\sum_{j=0}^{p} b_j x_{ij}\}}{1 + \sum_{j=0}^{p} b_j x_{ij}}, x_{i0} = 1.$$

Now $0 < P_i < 1$. Now,

$$1 - P_i = \frac{1}{1 + \exp\{\sum_j b_j x_{ij}\}}$$

$$\log\left(\frac{P_i}{1 - P_i}\right) = \sum_j b_j x_{ij}$$

where $\frac{P_i}{1-P_i} = e^{\sum b_j x_{ij}}$ equals to the odds for success. To find the mle of the $b_j's$ will be presented next. Suppose there are n patients. The likelihood function is

$$L = \prod_{i=1}^{n} P_i^{y_i}(1 - P_i)^{1-y_i} = \prod_{i=1}^{n}\left(\frac{P_i}{1 - P_i}\right)^{y_i}(1 - P_i) = \prod_{i=1}^{n} e^{y_i \sum_j b_j x_{ij}} \frac{1}{1 + \exp\{\sum_j b_j x_{ij}\}}.$$

Let $\sum_i y_i x_{ij} = t_j$. Then,

$$L = e^{\sum_j b_j t_j} \frac{1}{\prod_{i=1}^{n}\left[1 + \exp\{\sum_j b_j x_{ij}\}\right]}.$$

$$\log L = \sum_j b_j t_j - \sum \log[1 + \exp\{\sum_j b_j x_{ij}\}].$$

$$\frac{d \log L}{d\, b_k} = t_k - \sum \frac{x_{ik} \exp\{\sum_j b_j x_{ij}\}}{1 + \exp\{\sum_j b_j x_{ij}\}} = 0, k = 0, 1, 2, ..., p.$$

$$\frac{d^2 \log L}{d\, b_\ell b_k} = -\sum \frac{x_{i\ell} x_{ik} \exp\{\sum_j b_j x_{ij}\}}{1 + \exp\{\sum_j b_j x_{ij}\}}$$

The information function is

$$I_{\ell k} = -E\left(\frac{d^2 \log L}{d\, b_\ell d\, b_k}\right) = \sum \frac{x_{i\ell} x_{ik} \exp\{\sum_j b_j x_{ij}\}}{1 + \exp\{\sum_j b_j x_{ij}\}}$$

because the $x's$ are not random variables. $I = (I_{\ell k})_{p+1 \times p+1}$ $\widehat{I} = (I)_{b_j} = \widehat{b}_j = \left(I_{\ell k}(\widehat{b})\right)$. The confidence interval of b_j for large n is $\widehat{b}_j \pm z_{\alpha/2} s.e.(\widehat{b}_j)$ where $s.e.(\widehat{b}_j) = I_{jj}^{-1}(\widehat{b})$ which equals to the $(jj)^{th}$ element of $\widehat{I}^{-1}$. The null hypothesis is $H_0 : b_j = 0$. We can use the test statistic $z = \frac{\widehat{b}_j}{se(\widehat{b}_j)}$ or we can use the likelihood ratio test $-2 \log\left(\frac{\max_{H_0} L}{\max L}\right) \to \chi^2(1)$. Simulations show that the likelihood ratio test is better.

16.17.8 Chi Square Goodness of Fit Test

This test is due to Homshev and Lemashow. Suppose we have the following setup.

Patient No.	1	2	$\cdots$	n
$p_i = \widehat{P}_i$	p_1	p_2	$\cdots$	p_n
y_i	y_1	y_2	$\cdots$	y_n

i^{th} patient lies in class k if p_i lies in the k^{th} class. n_k equals to the number of subjects with p_i in the k^{th} class. O_k equals to the number of successes out of n_k $(y_i = 1)$ which equals to the number of observed successes in the k^{th} class. $E_k^* = \sum_{j \in A_k} P_j$, $A_k = k^{th}$ class. E_k equals to the estimated value of $E_k^* = \sum_{j \in A_k} p_j$.

$$X^2 = \sum_{k=1}^{g} \frac{(O_k - E_k)^2}{n_k \bar{p}_k (1 - \bar{p}_k)}, \ \ \bar{p}_k = \frac{E_k}{n_k}.$$

They claim that $X^2 \to \chi^2(g - 2)$.

Transform of Observed Variables in Logistic Regression

Example: This is Example 11.6 in the text book. It pertains to the treatment of cancer patients and the dose of the drug can cause CHF (congestive heart failure). z_1 is the dose level variable. z_2 is the QRS variable or the percent decrease in electrocardiographic. $x_1 = z_1 - \bar{z}$, $x_2 = z_2 - \bar{z}_2$, multiply $x_1 x_2$. $\log \frac{P_i}{1-P_i} = b_0 + b_1 x_{i1} + b_2 x_{i2} + b_3 x_{i1} x_{i2}$. The data is set up as

$$y_i = \begin{cases} 1, & \text{if no CHF.} \\ 0, & \text{otherwise.} \end{cases}$$

In the example, QRS is significant. The total dose level is not significant.

i	Variable	$\widehat{b}_i$	SE	$\widehat{b}_i/SE$
0	Constant	−3.757	1.576	−2.384*
1	QRS	0.254	0.102	2.480*
2	TD	−0.024	0.021	−1.160
3	TD*QRS	0.001	0.001	0.673

The measurements with the symbol '*' represent significant statistical results.

The final exam will be at 10:30am on December 12. It will be comprehensive and similar to the mid-term exam. You may bring a 3" × 5" note card with notes on both sides.

16.18 Homework 3 Goes Here

8. $x \sim lognormal(\mu, \sigma^2)$. $y = \log x \sim N(\mu, \sigma^2)$. $M_y(t) = E(e^{ty}) = e^{\mu t + \frac{\sigma^2 t^2}{2}}$. $E(x) = E(e^y) = M_y(1) = e^{\mu + \frac{\sigma^2}{2}}$. $E(x^2) = E(e^{2y}) = M_y(2) = e^{2\mu + 2\sigma^2}$. $\mu_x = e^{\mu + \frac{\sigma^2}{2}}$. $\sigma_x^2 = e^{2\mu + \sigma^2}(e^{\sigma^2} - 1)$. $\bar{y}$ and $s^2 = \frac{1}{n}\sum_{i=1}^n (y_i - \bar{y})^2$ are mle's for μ and σ^2. The mle for μ_x is $\widehat{\mu}_x = e^{\bar{x} + \frac{s^2}{2}}$. The mle for σ_x^2 is $\widehat{\sigma}_x^2 = e^{2\bar{x} + s^2}(e^{s^2} - 1)$.

   To find the bias. $E(\widehat{\mu}_x) = E\left[e^{\bar{x} + \frac{s^2}{2}}\right] = E\left[e^{\bar{x}}\right] E\left[e^{\frac{s^2}{2}}\right]$ because $\bar{x}$ and s^2 are independent. $\bar{x} \sim N(\mu, \sigma^2/n)$. $M_x(t) = e^{\mu + \frac{sigma^2}{2}\frac{t^2}{2}}$. So, $E(e^{\bar{x}}) = \mu_{\bar{x}}(1) = e^{\mu + \frac{\sigma^2}{2n}}$. $U = \frac{ns^2}{\sigma^2} \sim \chi^2(n-1)$. $M_U(t) = E(e^{tU}) = (1-2t)^{-\frac{n-1}{2}}$. $E(e^{\frac{s^2}{2}}) = E(e^{\frac{U\sigma^2}{2n}}) = (1 - \frac{\sigma^2}{n})^{-\frac{n-1}{2}}$. $E(\widehat{\sigma}_x^2) = E\left[e^{2\bar{x}}(e^{2s^2} - e^{s^2})\right] = E(e^{2\bar{x}}) \left[E(e^{2s^2}) - E(e^{s^2})\right]$.

16.19 References

1. Cox (1972), "Distribution Free Methods for Proportional Hazards and Related Regression Models." *Journal of Royal Stat Society,* Serv B, 34, p 187-202.

2. Kaplan and Meier (1958) *Journal of the American Statistical Association.*

Chapter 17

Modeling Project

Immudyne Project[1] Data Analysis

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Introduction

A known weight of powered yeast is treated with two factors: a disruption method(Factor A) and a digestion method(Factor B). The disruption method has three levels: A1) liquid nitrogen, A2) ground mechanically, and A3) unground (control). The digestion method has two levels: B1) water(H_2O), and B2) sodium hydroxide (NaOH). The purpose of treating the yeast is to break-up the cell walls of the yeast and to extract a compound called 1,3-beta-glucan [2] to be used in manufacturing makeup. Given this, the ideal method or combination of methods should produce the highest yield of 1,3-beta-glucan.

Yeast was exposed to each level of the two factors in the following manner: A1B1, A1B2, A2B1, A2B2, A3B1, A3B2. Thus, there are six treatments in this study, the yeast being the experimental unit. Yeast exposure to the treatments was replicated 3 times each. Measurements of the solution(in terms of area under the absorbance curve cm^2) occured at 5 minute intervals starting with 5 minutes and ending at 90 minutes. Thus, there are 18 measurements taken of each treatment per replication. This gives a total of $18(3) = 54$ measurements for each treatment and a total of $54(6) = 324$ measurements in the experiment. The questions to be answered are as follow:

1. Which disruption method(Factor A) is the most effective?
2. Which digestion method(Factor B) is the most effective?
3. Which of the factors or combination of factors produced the fastest rate of extraction?
4. What is the optimal extraction time?

[1] Center for Biotechnology, Old Dominion University
[2] Beta Glucan has been researched since the 1960's. It is extracted from baker's yeast cell walls. Historically 1,3-beta-glucan has been used to treat cancer by activating white blood cells. By activating the white blood cells, it enhances the body's immune system.

5. Are either of the two extraction methods more effective than the control?

Questions 1, 2, and 5 can definitely be answered with a statistical model. Consider time as another factor in the experiment, and Question 4 can be answered. However, Question 3 suggests finding the reaction rate of each treatment which would fall in the realm of Chemistry not Statistics. Moreover, the treatment with the fastest reaction rate does not necessarily imply the highest yield will be extracted. Question 3 will be omitted from the analysis.

17.1 Model Selection

Measurements were consistently taken from the same solution in time increments. This may lead to a repeated measures model depending on the correlation coefficient. Modeling the 18 time increments as another factor(Factor C) gives the following choice of models with possible interaction:

1. In the case that the correlation coefficient is *insignificant,* the data can be represented in a 3-way crossed design(ANOVA):

$$\left.\begin{aligned} y_{ijkm} = \quad & \mu + \alpha_i + \beta_j + \gamma_k + (\alpha\beta)_{ij} + (\alpha\gamma)_{ik} + \\ & (\beta\gamma)_{jk} + (\alpha\beta\gamma)_{ijk} + \epsilon_{ijkm}, \\ & i = 1,2,3; j = 1,2; k = 1,2,...,18; m = 1,2,3. \end{aligned}\right\} \tag{17.1}$$

   μ is the overall mean. α_i is the effect of the i-th level of Factor A. β_j is the effect of the j-th level of Factor B. γ_k is the effect of the k-th level of Factor C. $(\alpha\beta)_{ij}$ is the interaction of the i-th level of Factor A with the j-th level of Factor B. $(\alpha\gamma)_{ik}$ is the interaction of the i-th level of Factor A with the k-th level of Factor C. $(\beta\gamma)_{jk}$ is the interaction of the j-th level of Factor B with the k-th level of Factor C. $(\alpha\beta\gamma)_{ijk}$ is the interaction of the i-th level of Factor A, the j-th level of Factor B and the k-th level of Factor C. ϵ_{ijkm} is random error and $\epsilon \sim N(0, \sigma^2)$.

2. In the case that the correlation coefficient is *significant,* the data can be represented in a multivariate design(MANOVA) as:

$$\left.\begin{aligned} y_{ijk} = \quad & \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \epsilon_{ijk}, \\ & i = 1,2,3; j = 1,2; k = 1,...,18; \end{aligned}\right\} \tag{17.2}$$

   μ is the overall mean. α_i is mean effect of the i-th level of Factor A. β_j is the mean effect of the j-th level of Factor B. $(\alpha\beta)_{ij}$ is the mean effect of interaction between the i-th level of Factor A and the j-th level of Factor B. ϵ_{ijk} is random error and $\epsilon \sim N(0, \sigma^2 I)$.

Once the correlation coefficient has been quantified, the proper model can be selected and an analysis can be performed on the data.

17.1.1 Correlation Analysis

Eighteen dependent SAS variables, **Y1, Y2, ...,Y18,** were created to represent each measurement at time $i, i = 1,2,...,18$. Two independent SAS variables, **DISRUPT** and **DIGEST,** were created to represent Factor A and Factor B. A repeated measures analysis was performed to determine if correlation existed among the 18 dependent variables and to determine if the correlation was constant. Looking at a subset of the partial correlation matrix in Appendix A.2.1 on page 1182, it is obvious that the first 6 random variables are correlated(partial correlation was calculated for all 18 variables and all the partial correlations were high). Why only 6 variables appear on the printout will become apparent in the next paragraph. For now, it can be concluded that a model similar to equation 17.2 should be used.

The next problem is to determine if the correlation structure is constant. The sphericity test can be used to test for equal correlation among the 18 random variables. In a multivariate model, the hypotheses are $H_0 : \sigma^2 I$, versus H_1 : correlation is not equal(Λ.) Specifically with the given data, there were not enough degrees of freedom to run the sphericity test. However, if H_0 is rejected on some subset of the 18 random variables, then it can be concluded that H_1 is true. This approach gives enough degrees of freedom for the sphericity test. Since the p-value of the sphericity test on page 1182 in Appendix A.2.1 is 0.0000, reject H_0 using the subset **Y1, Y2, Y3, Y4, Y5, Y6.** ¿From this, it can be concluded that a different approach must be taken to analyze the data. PROC MIXED in SAS will be used.

17.2 Data Analysis

PROC MIXED gives many ways of choosing the structure for ϵ when $\epsilon \sim N(0, \Lambda)$. To analyze the data using PROC MIXED, a new data set was created. The dependent variable **Y** was created and the dependent variables **Y1–Y18** were dropped from the data set. **Y** is a 324×1 column vector containing all the information in **Y1–Y18.** AR(1) was used to model the correlation structure. The parameter estimate of the correlation is $\widehat{\rho} = 0.8922$ and the parameter estimate of σ^2 is $\widehat{\sigma}^2 = 1362.33$. PROC MIXED did give an estimate of ρ which PROC GLM did not do. The hypotheses tests in Appendix A.2.2 on pages 1183 and 1184 using PROC GLM match those in Appendix A.3.2 on page 1186 using PROC MIXED: the digestion methods and time levels are both significant, and the disruption methods are insignificant. The next problem is to determine which digestion level and which time level are most significant using PROC MIXED.

The disruption methods(Factor A) had an overall p-value of 0.0677. See Appendix A.3.2 on page 1186. None of the different levels of disruption are statistically significant at the 95% confidence level. So, the recommended disruption method is unground yeast.

The digestion methods(Factor B) had an overall p-value of 0.0001. See Appendix A.3.2 on page 1186. Digestion is a significant factor in the experiment. Using the Tukey pairwise comparison test, there is a statistically significant difference between H_2O and NaOH. See Appendix A.3.4 on page 1188. Since NaOH has the higher mean(255.305) compared to H_2O(118.765), use NaOH in the manufacturing process.

The time levels(Factor C) had an overall p-value of 0.0002. See Appendix A.3.2 on page 1186. Time is a significant factor in the experiment. Time level 16 resulted in the highest yield. Using the Tukey pairwise comparison test, time level 16 is statistically different from levels 1 thru 7. At time level 8, the yields become insignificant when compared with level 16. See Appendix A.3.4 on page 1188. Thus, use time level 8(40 minutes) in the manufacturing process.

17.2.1 Residual Analysis

The purpose of perfoming a residual analysis is the verify the normality assumption of the model. Since the residuals were correlated, they had to be transformed to make them uncorrelated. The transformation involved creating the 18×18 matrix $\widehat{V}$ such that $\widehat{V} = \widehat{\sigma}^2 \widehat{\rho}^{|i-j|}$, where $i = 1, 2, ..., 18$; $j = 1, 2, ..., 18$. Then, the following transformation matrix is derived:

$$\widehat{\Lambda}^{-1/2} = \left(I \otimes \widehat{V} \right)^{-1/2}.$$

$\otimes$ is the direct product of the 18×18 identity matrix I and $\widehat{V}$ and produces a 324×324 matrix. The transformed residuals are obtained by multiplying $\widehat{\Lambda}^{-1/2}$ by the residuals from PROC MIXED. The transformation matrix was created in PROC IML.

The hypotheses tests are: H_0 : uncorrelated residuals are normally distributed, vs H_1 : uncorrelated residuals are not normally distributed. Looking at Appendix A.3.5 on page 1189, the p-value of the Wilkins test for normality is 0.0001. Thus, reject H_0. The residuals do not come from a normal population. Looking at Appendix A.3.5 again, many of the extreme residuals came from the A2B2 treatment(ground yeast and NaOH).

17.3 Normality Remedy

Since many of the extreme residuals came from the A2B2 block, one or more of the replications from that block should removed. By trial and error, it was decided to remove the third replication. This still leaves two replications to estimate the mean response of the A2B2 treatment. Upon removing the third replication, the correlated residuals became normally distributed(Appendix A.4.6 on page 1197). However, the interaction[3] between Factor A(disruption) and Factor B(digestion) is now significant. The interaction between Factor B(digestion) and Factor C(time) is now significant. See Appendix A.4.1 on page 1191.

17.4 Re-Analysis of the Data

Currently, the model equation is similar to that of equation 2. The mean interaction responses are being estimated by :

$$\widehat{(\alpha\beta)}_{ij} = \bar{y}_{ij\cdot} - \bar{y}_{i\cdot\cdot} - \bar{y}_{\cdot j\cdot} + \bar{y}_{\cdot\cdot\cdot}.$$

The mean interaction responses should be estimated by:

$$\bar{y}_{ij\cdot} = \frac{1}{r}\sum_{k=1}^{r} y_{ijk}.$$

which corresponds to the following model $y_{ijk} = \mu_{ij} + \epsilon_{ijk}$. PROC MIXED was run again with just the interaction terms. The interaction means appear on pages 1193 and 1194 in Appendix A.4.3.

A Tukey pairwise comparison test(Appendix A.4.4 on page 1195) was run on the AB interaction. The highest mean occurred at the ground yeast and NaOH combination. The mean is 332.56, and the mean is statistically different from the other various combinations of each level of Factor A and Factor B. Thus, ground yeast in sodium hydroxide should be used in the manufacturing process.

A Tukey pairwise comparison test(Appendix A.4.5 on page 1196) was run on the BC interaction. The highest mean being 306.28 occurred at the NaOH level of Factor B and level 13 of Factor C. Holding NaOH constant, level 13 of Factor C is not statistically different from levels 9 thru 12 but is statistically different from levels 1 thru 8. The combination NaOH and level 9 of Factor C is statistically different from the H_2O level of Factor B and level 17 of Factor C. The yeast should be exposed to NaOH for 45 minutes.

17.5 Conclusions

1. Which disruption method(Factor A) is the most effective? Holding the digestion levels constant, there is a statistical significance and difference among the levels of the disruption methods at the 95% confidence level. Recommendation: ground yeast.

2. Which digestion method(Factor B) is the most effective? Holding the disruption levels constant, there is a statistical significance and difference between H_2O and NaOH at the 95% confidence level. Recommendation: NaOH(sodium hydroxide).

3. Which of the factors or combination of factors produced the fastest rate of extraction? Omitted.

4. What is the optimal extraction time? Holding the digestion levels constant, there is a statistical significance and difference between the various levels of time. Recommendation: 45 minutes.

5. Are either of the two extraction methods more effective than the control? Holding NaOH constant, ground yeast results in a statistically significant higher mean response than either unground yeast or yeast treated with liquid nitrogen. Holding H_2O constant, there is no statistical difference in the various levels of the extraction methods.

[3] As in the statistical sense: the level of one factor affects the mean response of another factor.

Appendix A

A.1 SAS Source Code

```
OPTIONS LS = 72;
DATA YEAST;
INFILE 'A:\DATA.TXT';
INPUT DISRUPT $ DIGEST $ Y1-Y18;


* PRINT THE DATA;


PROC PRINT;
VAR DISRUPT DIGEST Y1-Y18;
TITLE 'IMMUDYNE PROJECT';
TITLE2 'RAW DATA OF 1,3-BETA-GLUCAN';
RUN;


* REPEATED MEASURES MODEL;

PROC GLM;
CLASS DISRUPT DIGEST;
MODEL Y1-Y18 = DIGEST | DISRUPT/NOUNI;
REPEATED TIME 18 (5 10 15 20 25 30 35 40 45 50
                  55 60 65 70 75 80 85 90)/PRINTE;
TITLE 'IMMUDYNE PROJECT';
TITLE2 'GLM ANALYSIS OF THE DATA';
RUN;

* RUN THE SPHERICITY TEST;

PROC GLM;
CLASS DISRUPT DIGEST;
MODEL Y1-Y6 = DIGEST | DISRUPT/NOUNI;
REPEATED TIME 6/PRINTE;
TITLE 'IMMUDYNE PROJECT';
TITLE2 'GLM ANALYSIS OF THE DATA/SPHERICITY TEST';
RUN;
```

```
* CREATE A NEW DATA SET TO USE WITH PROC MIXED;

DATA NEW1; SET YEAST;
ARRAY T{18} Y1-Y18;
YEAST+1;
DO TIME = 1 TO 18;
   Y=T{TIME};
OUTPUT;
END;
DROP Y1-Y18;


* MODEL THE CORRELATION STRUCTURE;

PROC MIXED DATA = NEW1 METHOD = REML;
CLASS YEAST DIGEST DISRUPT TIME;
MODEL Y = DIGEST | DISRUPT | TIME /CHISQ PREDICTED;
REPEATED /TYPE = AR(1) SUBJECT = YEAST R;
LSMEANS DISRUPT DIGEST TIME/ADJUST=TUKEY;
MAKE 'PREDICTED' OUT=NEW2 noprint;
TITLE 'IMMUDYNE PROJECT';
TITLE2 'DATA ANALYSIS WITH PROC MIXED';
RUN;


* UN-CORRELATE THE RESIDUALS;

PROC IML;

        START XFORM;
        USE NEW2;
        READ ALL;

        I18 = I(18);
        HATV = J(18, 18, 0);
        SIGMAH = J(324, 324, 0);
        U = J(324, 1, 0);

        DO I = 1 TO 18 BY 1;
           DO J = 1 TO 18 BY 1;
                HATV[I,J] = 1362.326*(0.8922)**(ABS(I-J));
           END;
        END;

        SIGMAH = I18 @ HATV;
        SIGMAH = SQRT(SIGMAH);
        SIGMAH = INV(SIGMAH);
        U = SIGMAH*RESID;

        CREATE NEW3 VAR{U};
        APPEND;
        SHOW CONTENTS;

FINISH XFORM;
```

```
RUN XFORM;


PROC UNIVARIATE DATA = NEW3 PLOT NORMAL;
VAR U;
TITLE 'IMMUDYNE PROJECT';
TITLE2 'UN-CORRELATED RESIDUAL ANALYSIS';
RUN;

PROC UNIVARIATE DATA = NEW2 PLOT NORMAL;
VAR RESID;
TITLE 'IMMUDYNE PROJECT';
TITLE2 'CORRELATED RESIDUAL ANALYSIS';
RUN;

* REMOVE THE 3-RD REPLICATION FROM THE A2B2 BLOCK;

DATA YEAST; SET YEAST;
IF _N_ = 18 THEN DELETE;


* PRINT THE DATA;


PROC PRINT DATA = YEAST;
VAR DISRUPT DIGEST Y1-Y18;
RUN;




DATA FINAL; SET YEAST;

ARRAY T{18} Y1-Y18;
YEAST+1;
DO TIME = 1 TO 18;
   Y=T{TIME};
OUTPUT;
END;
DROP Y1-Y18;
RUN;

RUN;

* MODEL THE REDUCED DATA SET;

PROC MIXED DATA = FINAL METHOD = REML;
CLASS YEAST DISRUPT DIGEST TIME;
MODEL Y = DISRUPT | DIGEST | TIME /CHISQ PREDICTED S;
*LSMEANS DISRUPT | DIGEST | TIME /ADJUST=TUKEY;
MAKE 'PREDICTED' OUT=NEW4 noprint;
REPEATED /TYPE = AR(1) SUBJECT = YEAST R;
TITLE 'IMMUDYNE PROJECT';
TITLE2 'ANALYSIS ON THE REDUCED DATA SET';
```

```
RUN;



*MODEL THE INTERACTION TERMS ONLY;


PROC MIXED DATA = FINAL METHOD = REML;
CLASS YEAST DISRUPT DIGEST TIME;
MODEL Y = DISRUPT*DIGEST DIGEST*TIME /CHISQ PREDICTED S;
LSMEANS DISRUPT*DIGEST DIGEST*TIME /ADJUST=TUKEY;
MAKE 'PREDICTED' OUT=NEW4 noprint;
REPEATED /TYPE = AR(1) SUBJECT = YEAST R;
TITLE 'IMMUDYNE PROJECT';
TITLE2 'ANALYSIS OF INTERACTION TERMS ONLY';
RUN;

* UN-CORRELATE THE RESIDUALS;

PROC IML;

        START XFORM;
        USE NEW4;
        READ ALL;

        I18 = I(18);
        HATV = J(17, 18, 0);
        SIGMAH = J(306, 306, 0);
        TEMP = J(306, 324, 0);
        U = J(324, 1, 0);

        DO I = 1 TO 17 BY 1;
           DO J = 1 TO 18 BY 1;
                HATV[I,J] = 556.43*(0.727)**(ABS(I-J));
           END;
        END;

        TEMP = I18 @ HATV;

        * THE LAST 18 COLUMNS ARE JUNK;
        * OMIT THE LAST 18 COLUMNS;

        DO I = 1 TO 306 BY 1;
          DO J = 1 TO 306 BY 1;
             SIGMAH[I,J] = TEMP[I,J];
          END;
        END;

        SIGMAH = SQRT(SIGMAH);
        SIGMAH = GINV(SIGMAH);
        U = SIGMAH*RESID;

        CREATE NEW5 VAR{U};
```

```
        APPEND;
        SHOW CONTENTS;

FINISH XFORM;
RUN XFORM;



* TRANSFORMED RESIDUAL ANALYSIS;

PROC UNIVARIATE DATA=NEW5 PLOT NORMAL;
VAR U;
TITLE 'IMMUDYNE PROJECT';
TITLE2 'UN-CORRELATED RESIDUAL ANALYSIS';
RUN;


PROC UNIVARIATE DATA=NEW4 PLOT NORMAL;
VAR RESID;
TITLE 'IMMUDYNE PROJECT';
TITLE2 'CORRELATED RESIDUAL ANALYSIS';
RUN;
```

A.2 Repeated Measures Analysis using PROC GLM

A.2.1 Selected Partial Correlation Coefficients

```
General Linear Models Procedure
Repeated Measures Analysis of Variance

Partial Correlation Coefficients from the Error SS&CP Matrix / Prob > |r|
```

DF = 12	Y1	Y2	Y3	Y4	Y5	Y6
Y1	1.000000	0.805055	0.684215	0.797613	0.739900	0.779293
	0.0001	0.0009	0.0099	0.0011	0.0038	0.0017
Y2	0.805055	1.000000	0.910334	0.959974	0.967580	0.951462
	0.0009	0.0001	0.0001	0.0001	0.0001	0.0001
Y3	0.684215	0.910334	1.000000	0.924955	0.945084	0.932897
	0.0099	0.0001	0.0001	0.0001	0.0001	0.0001
Y4	0.797613	0.959974	0.924955	1.000000	0.974034	0.931556
	0.0011	0.0001	0.0001	0.0001	0.0001	0.0001
Y5	0.739900	0.967580	0.945084	0.974034	1.000000	0.952571
	0.0038	0.0001	0.0001	0.0001	0.0001	0.0001
Y6	0.779293	0.951462	0.932897	0.931556	0.952571	1.000000
	0.0017	0.0001	0.0001	0.0001	0.0001	0.0001

Highly correlated. So were the other 12 variables.

```
Test for Sphericity:  Mauchly's Criterion = 0.0066855
Chisquare Approximation = 50.57899 with 14 df Prob > Chisquare = 0.0000
```

$H_0 : \sigma^2 I$
$H_1 : \Lambda$.
$\Rightarrow$ reject H_0.

A.2.2 Hypotheses Tests

```
                      General Linear Models Procedure
                          Class Level Information

                     Class    Levels    Values
                     DISRUPT       3    GROUND LN2 UNGROUND
                     DIGEST        2    H2O NAOH

                    Number of observations in data set = 18

                      General Linear Models Procedure
                   Repeated Measures Analysis of Variance
                    Repeated Measures Level Information

Dependent Variable          Y1       Y2       Y3       Y4       Y5       Y6       Y7       Y8
     Level of TIME           5       10       15       20       25       30       35       40

Dependent Variable          Y9      Y10      Y11      Y12      Y13      Y14      Y15      Y16
     Level of TIME          45       50       55       60       65       70       75       80

Dependent Variable         Y17      Y18
     Level of TIME          85       90

                      General Linear Models Procedure
                   Repeated Measures Analysis of Variance
             Tests of Hypotheses for Between Subjects Effects

Source                  DF             Type III SS            Mean Square   F Value      Pr > F

DIGEST                   1        1510092.93175021       1510092.93175021     68.46      0.0001

DISRUPT                  2          93660.91046843         46830.45523421      2.12      0.1624
DISRUPT*DIGEST           2          73718.67333538         36859.33666769      1.67      0.2290

Error                   12         264697.51683458         22058.12640288
```

```
                    General Linear Models Procedure
                  Repeated Measures Analysis of Variance
          Univariate Tests of Hypotheses for Within Subject Effects

Source: TIME
                                                              Adj  Pr > F
    DF          Type III SS          Mean Square     F Value     Pr > F     G - G      H - F
    17       148365.0545959         8727.3561527       38.55     0.0001    0.0001     0.0001

Source: TIME*DIGEST
                                                              Adj  Pr > F
    DF          Type III SS          Mean Square     F Value     Pr > F     G - G      H - F
    17        37511.9907485         2206.5876911        9.75     0.0001    0.0001     0.0001


Source: TIME*DISRUPT
                                                              Adj  Pr > F
    DF          Type III SS          Mean Square     F Value     Pr > F     G - G      H - F
    34         6918.3772001          203.4816824        0.90     0.6324    0.5285     0.5851

Source: TIME*DISRUPT*DIGEST
                                                              Adj  Pr > F
    DF          Type III SS          Mean Square     F Value     Pr > F     G - G      H - F
    34         6568.0519730          193.1779992        0.85     0.7019    0.5660     0.6397

Source: Error(TIME)

    DF          Type III SS          Mean Square
   204        46181.3002023          226.3789226

                    Greenhouse-Geisser Epsilon = 0.2480
                           Huynh-Feldt Epsilon = 0.5585
```

A.3 Repeated Measures Analysis using PROC MIXED

A.3.1 Estimates of ρ and σ^2

```
                 Covariance Parameter Estimates (REML)

Cov Parm            Ratio      Estimate     Std Error       Z  Pr > |Z|

DIAG AR(1)     0.00065491    0.89220563    0.02574286   34.66    0.0001
Residual       1.00000000  1362.3260943  318.03926192    4.28    0.0001


          Model Fitting Information for Y

Description                        Value
Observations                    324.0000
Variance Estimate               1362.326
Standard Deviation Estimate      36.9097
REML Log Likelihood             -983.088
Akaike's Information Criterion  -985.088
Schwarz's Bayesian Criterion    -988.463
-2 REML Log Likelihood          1966.176
Null Model LRT Chi-Square       336.1816
Null Model LRT DF                 1.0000
Null Model LRT P-Value            0.0000
```

A.3.2 Tests of Hypotheses

Tests of Fixed Effects

Source	NDF	DDF	Type III ChiSq	Type III F	Pr > ChiSq	Pr > F
DIGEST	1	12	109.56	109.56	0.0001	0.0001
DISRUPT	2	12	6.80	3.40	0.0334	0.0677
DIGEST*DISRUPT	2	12	5.35	2.67	0.0690	0.1095
TIME	17	204	48.67	2.86	0.0001	0.0002
DIGEST*TIME	17	204	26.86	1.58	0.0601	0.0718
DISRUPT*TIME	34	204	33.03	0.97	0.5148	0.5187
DIGEST*DISRUPT*TIME	34	204	34.86	1.03	0.4270	0.4374

A.3.3 Least Squares Means

Least Squares Means

Level	LSMEAN	Std Error	DDF	T	Pr > |T|
DISRUPT GROUND	207.13302148	11.29689462	12	18.34	0.0001
DISRUPT LN2	188.41610907	11.29689462	12	16.68	0.0001
DISRUPT UNGROUND	165.55494593	11.29689462	12	14.65	0.0001
DIGEST H2O	118.76478185	9.22387583	12	12.88	0.0001
DIGEST NAOH	255.30460247	9.22387583	12	27.68	0.0001
TIME 1	147.26801167	8.69970017	204	16.93	0.0001
TIME 2	152.62652444	8.69970017	204	17.54	0.0001
TIME 3	158.16350278	8.69970017	204	18.18	0.0001
TIME 4	164.35957389	8.69970017	204	18.89	0.0001
TIME 5	171.29198056	8.69970017	204	19.69	0.0001
TIME 6	176.52320667	8.69970017	204	20.29	0.0001
TIME 7	179.44056111	8.69970017	204	20.63	0.0001
TIME 8	182.58687500	8.69970017	204	20.99	0.0001
TIME 9	185.44511056	8.69970017	204	21.32	0.0001
TIME 10	187.36433667	8.69970017	204	21.54	0.0001
TIME 11	196.97766333	8.69970017	204	22.64	0.0001
TIME 12	200.23405278	8.69970017	204	23.02	0.0001
TIME 13	210.38874167	8.69970017	204	24.18	0.0001
TIME 14	210.22912889	8.69970017	204	24.17	0.0001
TIME 15	206.52012778	8.69970017	204	23.74	0.0001
TIME 16	214.74531333	8.69970017	204	24.68	0.0001
TIME 17	214.07752778	8.69970017	204	24.61	0.0001
TIME 18	208.38222000	8.69970017	204	23.95	0.0001

A.3.4 Tukey Pairwise Comparisons

Means

Level 1	Level 2	Difference	Std Error	DDF	T	Pr > |T|	Adjustment	Adj P
GROUND	LN2	18.71691241	15.97622158	12	1.17	0.2641	Tukey	0.4913
GROUND	UNGROUND	41.57807556	15.97622158	12	2.60	0.0231	Tukey	0.0561
LN2	UNGROUND	22.86116315	15.97622158	12	1.43	0.1780	Tukey	0.3568
H2O	NAOH	-136.5398206	13.04453030	12	-10.47	0.0001	Tukey	0.0000

Level 1	Level 2	Difference	Std Error	DDF	T	Pr > |T|	Adjustment	Adj P
TIME 1	TIME 16	-67.47730167	11.13625000	204	-6.06	0.0001	Tukey-Kramer	0.0000
TIME 2	TIME 16	-62.11878889	10.98686818	204	-5.65	0.0001	Tukey-Kramer	0.0000
TIME 3	TIME 16	-56.58181056	10.81698679	204	-5.23	0.0001	Tukey-Kramer	0.0001
TIME 4	TIME 16	-50.38573944	10.62335239	204	-4.74	0.0001	Tukey-Kramer	0.0005
TIME 5	TIME 16	-43.45333278	10.40204033	204	-4.18	0.0001	Tukey-Kramer	0.0055
TIME 6	TIME 16	-38.22210667	10.14825521	204	-3.77	0.0002	Tukey-Kramer	0.0237
TIME 7	TIME 16	-35.30475222	9.85604464	204	-3.58	0.0004	Tukey-Kramer	0.0431
TIME 8	TIME 16	-32.15843833	9.51787324	204	-3.38	0.0009	Tukey-Kramer	0.0792
TIME 9	TIME 16	-29.30020278	9.12395985	204	-3.21	0.0015	Tukey-Kramer	0.1252
TIME 10	TIME 16	-27.38097667	8.66118801	204	-3.16	0.0018	Tukey-Kramer	0.1424
TIME 11	TIME 16	-17.76765000	8.11118518	204	-2.19	0.0296	Tukey-Kramer	0.7575
TIME 12	TIME 16	-14.51126056	7.44660629	204	-1.95	0.0527	Tukey-Kramer	0.8891
TIME 13	TIME 16	-4.35657167	6.62294373	204	-0.66	0.5114	Tukey-Kramer	1.0000
TIME 14	TIME 16	-4.51618444	5.55650223	204	-0.81	0.4173	Tukey-Kramer	1.0000
TIME 15	TIME 16	-8.22518556	4.03940434	204	-2.04	0.0430	Tukey-Kramer	0.8479

A.3.5 Residual Analysis

```
                          Univariate Procedure

Variable=U

                 Moments

N                324  Sum Wgts        324
Mean               0  Sum               0
Std Dev     5.519142  Variance   30.46093
Skewness    0.117602  Kurtosis   9.038323
USS         9838.879  CSS        9838.879
CV                 .  Std Mean   0.306619
T:Mean=0           0  Pr>|T|       1.0000
Num ^= 0         324  Num > 0         170
M(Sign)            8  Pr>=|M|      0.4047
Sgn Rank         337  Pr>=|S|      0.8421
```

W:Normal 0.907035 Pr<W 0.0001 } H_0 : Normally distributed. H_1 : Not. $\Rightarrow$ reject H_0.

```
              Quantiles(Def=5)

100% Max  34.20967       99%  16.31307
75% Q3     2.3683       95%  7.481788
50% Med   0.12592       90%  5.313722
25% Q1   -2.38169       10%  -5.36281
0% Min  -27.3134        5%  -7.21337
1%  -15.9949
Range     61.52305
Q3-Q1     4.749986
                 Mode      -27.3134
```

```
                          Extremes

                 Lowest    Obs     Highest    Obs
                -27.3134(     303) 13.30007(     178)
                -26.8752(     286) 16.31307(     285)
                -20.3073(     305) 16.97437(     125)
                -15.9949(     124) 23.61644(     287)
                -15.9366(     176) 34.20967(     304)


                      Univariate Procedure

Variable=U

                   Histogram                          #      Boxplot
   32.5+*                                              1         *
       .
       .*                                              1         *
       .*                                              2         0
       .**                                             5         0
       .**********                                    28         |
    2.5+*********************************************  133      +--+--+
       .****************************************      118      +-----+
       .*********                                     25         |
       .**                                             6         0
       .*                                              2         0
       .*                                              1         *
  -27.5+*                                              2         *
        ----+----+----+----+----+----+----+----+----
        * may represent up to 3 counts
```

A.4 Analysis with the Unbalanced Data Set

A.4.1 Tests of Hypotheses

Tests of Fixed Effects

Source	NDF	DDF	Type III ChiSq	Type III F	Pr > ChiSq	Pr > F
DIGEST	1	11	487.63	487.63	0.0001	0.0001
DISRUPT	2	11	54.25	27.13	0.0001	0.0001
DIGEST*DISRUPT	2	11	49.15	24.57	0.0001	0.0001
TIME	17	187	92.36	5.43	0.0001	0.0001
DIGEST*TIME	17	187	42.96	2.53	0.0005	0.0012
DISRUPT*TIME	34	187	38.88	1.14	0.2593	0.2824
DIGEST*DISRUPT*TIME	34	187	39.52	1.16	0.2368	0.2611

A.4.2 Estimates Fitting $y_{ijk} = \mu_{ij} + \epsilon_{ijk}$

Covariance Parameter Estimates (REML)

Cov Parm	Ratio	Estimate	Std Error	Z	Pr > |Z|
DIAG AR(1)	0.00130647	0.72696144	0.04489917	16.19	0.0001
Residual	1.00000000	556.43333739	89.18816630	6.24	0.0001

Model Fitting Information for Y

Description	Value
Observations	306.0000
Variance Estimate	556.4333
Standard Deviation Estimate	23.5888
REML Log Likelihood	-1164.41
Akaike's Information Criterion	-1166.41
Schwarz's Bayesian Criterion	-1169.99
-2 REML Log Likelihood	2328.813
Null Model LRT Chi-Square	170.7341
Null Model LRT DF	1.0000
Null Model LRT P-Value	0.0000

A.4.3 Least Squares Means of Interaction Terms Only

Least Squares Means

Level	LSMEAN	Std Error	DDF	T	Pr > |T|
DISRUPT*DIGEST GROUND H2O	117.36752850	7.17953069	12	16.35	0.0001
DISRUPT*DIGEST GROUND NAOH	332.55973756	8.76639565	12	37.94	0.0001
DISRUPT*DIGEST LN2 H2O	126.93807250	7.17953069	12	17.68	0.0001
DISRUPT*DIGEST LN2 NAOH	253.82989140	7.19040521	12	35.30	0.0001
DISRUPT*DIGEST UNGROUND H2O	111.98874456	7.17953069	12	15.60	0.0001
DISRUPT*DIGEST UNGROUND NAOH	219.28976503	7.19040521	12	30.50	0.0001
DIGEST*TIME H2O 1	103.78572333	7.86294642	254	13.20	0.0001
DIGEST*TIME H2O 2	103.23852667	7.86294642	254	13.13	0.0001
DIGEST*TIME H2O 3	103.65090556	7.86294642	254	13.18	0.0001
DIGEST*TIME H2O 4	108.95637000	7.86294642	254	13.86	0.0001
DIGEST*TIME H2O 5	107.01341667	7.86294642	254	13.61	0.0001
DIGEST*TIME H2O 6	107.53683556	7.86294642	254	13.68	0.0001
DIGEST*TIME H2O 7	113.04025556	7.86294642	254	14.38	0.0001
DIGEST*TIME H2O 8	112.58853889	7.86294642	254	14.32	0.0001
DIGEST*TIME H2O 9	115.09454333	7.86294642	254	14.64	0.0001
DIGEST*TIME H2O 10	113.04847333	7.86294642	254	14.38	0.0001
DIGEST*TIME H2O 11	118.35393778	7.86294642	254	15.05	0.0001
DIGEST*TIME H2O 12	120.53481667	7.86294642	254	15.33	0.0001
DIGEST*TIME H2O 13	127.45018333	7.86294642	254	16.21	0.0001
DIGEST*TIME H2O 14	129.71826889	7.86294642	254	16.50	0.0001
DIGEST*TIME H2O 15	135.03167778	7.86294642	254	17.17	0.0001
DIGEST*TIME H2O 16	138.67174889	7.86294642	254	17.64	0.0001
DIGEST*TIME H2O 17	144.11995556	7.86294642	254	18.33	0.0001
DIGEST*TIME H2O 18	135.93189556	7.86294642	254	17.29	0.0001

Least Squares Means

Level	LSMEAN	Std Error	DDF	T	Pr > |T|
DIGEST*TIME NAOH 1	201.84637995	8.38168934	254	24.08	0.0001
DIGEST*TIME NAOH 2	212.45982995	8.38168934	254	25.35	0.0001
DIGEST*TIME NAOH 3	224.61384245	8.38168934	254	26.80	0.0001
DIGEST*TIME NAOH 4	229.83536745	8.38168934	254	27.42	0.0001
DIGEST*TIME NAOH 5	246.67845495	8.38168934	254	29.43	0.0001
DIGEST*TIME NAOH 6	259.42170495	8.38168934	254	30.95	0.0001
DIGEST*TIME NAOH 7	258.76501745	8.38168934	254	30.87	0.0001
DIGEST*TIME NAOH 8	265.25200495	8.38168934	254	31.65	0.0001
DIGEST*TIME NAOH 9	271.52601745	8.38168934	254	32.40	0.0001
DIGEST*TIME NAOH 10	276.61975495	8.38168934	254	33.00	0.0001
DIGEST*TIME NAOH 11	292.97327995	8.38168934	254	34.95	0.0001
DIGEST*TIME NAOH 12	293.85330495	8.38168934	254	35.06	0.0001
DIGEST*TIME NAOH 13	306.27707995	8.38168934	254	36.54	0.0001
DIGEST*TIME NAOH 14	302.39020495	8.38168934	254	36.08	0.0001
DIGEST*TIME NAOH 15	292.06071745	8.38168934	254	34.85	0.0001
DIGEST*TIME NAOH 16	305.15894245	8.38168934	254	36.41	0.0001
DIGEST*TIME NAOH 17	299.37300495	8.38168934	254	35.72	0.0001
DIGEST*TIME NAOH 18	294.97145495	8.38168934	254	35.19	0.0001

A.4.4 Tukey Pairwise Comparisons of the AB Interaction Terms

Differences of Least Squares Means

Level 1	Level 2	Difference	Std Error	DDF	T	Pr > |T|	Adjustment	Adj P
GROUND H2O	GROUND NAOH	-215.1922091	11.33116735	12	-18.99	0.0001	Tukey-Kramer	0.0000
GROUND H2O	LN2 H2O	-9.57054399	10.02950959	12	-0.95	0.3588	Tukey-Kramer	0.9239
GROUND H2O	LN2 NAOH	-136.4623629	10.16108203	12	-13.43	0.0001	Tukey-Kramer	0.0000
GROUND H2O	UNGROUND H2O	5.37878395	10.02950959	12	0.54	0.6016	Tukey-Kramer	0.9934
GROUND H2O	UNGROUND NAOH	-101.9222365	10.16108203	12	-10.03	0.0001	Tukey-Kramer	0.0000
GROUND NAOH	LN2 H2O	205.62166507	11.33116735	12	18.15	0.0001	Tukey-Kramer	0.0000
GROUND NAOH	LN2 NAOH	78.72984616	11.21333262	12	7.02	0.0001	Tukey-Kramer	0.0001
GROUND NAOH	UNGROUND H2O	220.57099301	11.33116735	12	19.47	0.0001	Tukey-Kramer	0.0000
GROUND NAOH	UNGROUND NAOH	113.26997253	11.21333262	12	10.10	0.0001	Tukey-Kramer	0.0000
LN2 H2O	LN2 NAOH	-126.8918189	10.16108203	12	-12.49	0.0001	Tukey-Kramer	0.0000
LN2 H2O	UNGROUND H2O	14.94932794	10.02950959	12	1.49	0.1619	Tukey-Kramer	0.6761
LN2 H2O	UNGROUND NAOH	-92.35169254	10.16108203	12	-9.09	0.0001	Tukey-Kramer	0.0000
LN2 NAOH	UNGROUND H2O	141.84114685	10.16108203	12	13.96	0.0001	Tukey-Kramer	0.0000
LN2 NAOH	UNGROUND NAOH	34.54012637	10.02950959	12	3.44	0.0049	Tukey-Kramer	0.0434
UNGROUND H2O	UNGROUND NAOH	-107.3010205	10.16108203	12	-10.56	0.0001	Tukey-Kramer	0.0000

A.4.5 Tukey Pairwise Comparisons of the BC Interaction Terms

Differences of Least Squares Means

Level 1	Level 2	Difference	Std Error	DDF	T	Pr > |T|	Adjustment	Adj P
NAOH 1	NAOH 13	-104.4307000	11.66524780	254	-8.95	0.0001	Tukey-Kramer	0.0000
NAOH 2	NAOH 13	-93.81725000	11.61636126	254	-8.08	0.0001	Tukey-Kramer	0.0000
NAOH 3	NAOH 13	-81.66323750	11.54877537	254	-7.07	0.0001	Tukey-Kramer	0.0000
NAOH 4	NAOH 13	-76.44171250	11.45515346	254	-6.67	0.0001	Tukey-Kramer	0.0000
NAOH 5	NAOH 13	-59.59862500	11.32510371	254	-5.26	0.0001	Tukey-Kramer	0.0002
NAOH 6	NAOH 13	-46.85537500	11.14372920	254	-4.20	0.0001	Tukey-Kramer	0.0163
NAOH 7	NAOH 13	-47.51206250	10.88929750	254	-4.36	0.0001	Tukey-Kramer	0.0089
NAOH 8	NAOH 13	-41.02507500	10.52926332	254	-3.90	0.0001	Tukey-Kramer	0.0481
NAOH 9	NAOH 13	-34.75106250	10.01287429	254	-3.47	0.0006	Tukey-Kramer	0.1703
NAOH 10	NAOH 13	-29.65732500	9.25558054	254	-3.20	0.0015	Tukey-Kramer	0.3206
NAOH 11	NAOH 13	-13.30380000	8.09897181	254	-1.64	0.1017	Tukey-Kramer	0.9997
NAOH 12	NAOH 13	-12.42377500	6.16294890	254	-2.02	0.0449	Tukey-Kramer	0.9889

A.4.6 Correlated Residual Analysis

```
                          Univariate Procedure

Variable=RESID         Residual

                Moments

N                306  Sum Wgts        306
Mean               0  Sum               0
Std Dev     21.06598  Variance   443.7754
Skewness    -0.17742  Kurtosis    0.34105
USS         135351.5  CSS        135351.5
CV                 .  Std Mean   1.204262
T:Mean=0           0  Pr>|T|       1.0000
Num ^= 0         306  Num > 0         157
M(Sign)            4  Pr>=|M|      0.6891
Sgn Rank       435.5  Pr>=|S|      0.7791
```

$$\texttt{W:Normal 0.990468 Pr<W 0.9528}\ \left.\right\}\ \begin{array}{l} H_0 : \text{Normally distributed.}\\ H_1 : \text{Not.}\\ \Rightarrow\ \text{accept } H_0. \end{array}$$

```
W:Normal   0.990468  Pr<W         0.9528

          Quantiles(Def=5)

100% Max  72.24006       99%  46.36316
75%  Q3   14.76201       95%  31.56615
50%  Med  0.280578       90%  24.28432
25%  Q1   -13.6608       10%  -27.2872
0%   Min   -68.681        5%  -34.3395
                          1%  -51.8734
Range      140.921
Q3-Q1     28.42282
Mode       -68.681
```

```
                  Extremes

Lowest    Obs     Highest    Obs
 -68.681(     303) 42.77665(     162)
-63.6405(     305) 46.36316(     284)
-59.9489(     306) 48.81099(     159)
-51.8734(     289) 48.99876(     278)
-48.0589(     124) 72.24006(     287)


                          Univariate Procedure

Variable=RESID         Residual

                     Histogram                  #             Boxplot
          75+*                                  1                0
            .
            .
            .***                                5                |
            .******                            12                |
            .******************                36                |
            .************************          48             +-----+
           5+****************************      55             *--+--*
            .*************************         50             |     |
            .***********************           46             +-----+
            .**************                    27                |
            .*********                         17                |
            .***                                5                |
            .*                                  2                0
         -65+*                                  2                0
             ----+----+----+----+----+---
             * may represent up to 2 counts
```

Index

Index